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Coupling agricultural plant growth and hydrological models for climate change projections

Dissertation
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Abstract

The continuous increase of the greenhouse gas carbon dioxide (CO_2) is expected to impact a wide range of processes within the soil-plant system, including biomass production and transpiration. In C3 and C4 plants, elevated CO_2 (eCO_2) is reported to decrease stomatal conductance which in turn reduces water loss through transpiration at the leaf level. However, eCO_2 is observed to increase biomass production of C3 plants, which might counteract the water saving effect at the canopy level by increased leaf area. The direct CO_2-fertilizating effect is not observed for C4 plants, but a combination of eCO_2 and drought stress has been observed to distinctly increase C4 biomass. Free-air carbon dioxide enrichment (FACE) experiments have been developed to investigate the effect of eCO_2 on the soil-plant system under field conditions providing a number of parameters valuable for crop modelling. Process-based models, which are used to project climate change effects on agricultural systems, need to be capable of simulating the effects observed in the field. However, recent crop model ensemble studies revealed strong limitations, for instance in simulating the distinct biomass increase of the C4 crop maize under eCO_2 and water stress. To improve the representation of the dynamic behavior of the soil-plant system, two independent process-based models with a high degree of process representation, i.e. a plant growth and a soil hydrological model, were coupled in this work, and straightforward CO_2 response functions regulating stomatal conductance and biomass accumulation were implemented. A comprehensive parameter uncertainty analysis based on Latin Hypercube sampling has been undertaken for the established model. The coupled model was applied to long-term data of a FACE experiment on a temperate C3 grassland. Results imply that temperate, mown, wet-dry C3 grasslands could benefit from biomass increase while maintaining water consumption, already with a modest increase of CO_2 concentration of 20%. Further, the expected water saving effect at the leaf level could be offset at a stand level as a result of increased transpiration, caused by a biomass gain under eCO_2. For simulating the combined effect of eCO_2 and water stress on C4 crops, the coupled model was applied to a two-year long FACE experiment where maize was grown under combined eCO_2 and water limited conditions. The clear benefit of maize biomass from eCO_2 under water-limited conditions was well simulated. Results indicate that the coupled hydrological-plant growth model is capable of simulating the relevant climate change feedback mechanisms on plant growth of C4 plants. The obtained values of calibrated response parameters could be used in other crop models to project maize yields under climate change conditions. Based on the results of this work, the importance of plant-specific CO_2 response factors obtained by using comprehensive FACE data is emphasized. Further, for the rigorous assessment of crop models and their applicability to project yields and water fluxes under climate change, datasets that go beyond single criteria (only biomass response) and single effects (only eCO_2) are needed.

Table of Contents

List of Tables

List of Figures

1 Extended Summary

1.1 Introduction

1.1.1 Climate change effects on agricultural systems

The concentration of atmospheric carbon dioxide (CO_2) is projected to increase from preindustrial 280 ppm to about 700-900 ppm at the end of 21st century (Pachauri et al., 2014). The rise of CO_2 is known to affect a large number of processes within the soil-plant system (Ainsworth and Long, 2005). The effect might vary among plant groups, e.g. C3 and C4 plants, in particular evapotranspiration and biomass accumulation are affected. According to Long et al. (2004) two essential responses build the basis for the effects of elevated CO_2 (eCO_2) on plants and ecosystems: a reduction of stomatal conductance and an enhancement of photosynthesis of C3 plants under eCO_2. The decrease of stomatal conductance is caused by increased stomatal closure which in turn results in reduced water loss, i.e. transpiration, on the leaf level (Ainsworth and Rogers, 2007). At the same time, C3 plants (e.g. wheat, ryegrass, barley) show an increased photosynthesis caused by an accelerated CO_2 assimilation rate, which leads to a higher biomass production. This increased biomass accumulation is linked to a higher leaf area index, which in turn might increase transpiration on a canopy level (Manea and Leishman, 2014; Tor-ngern et al., 2015). In contrast to C3 plants, the photosynthesis of C4 plants (e.g. sorghum and maize) is already saturated under ambient CO_2 (aCO_2) concentration (Ghannoum et al., 2000). However, C4 crops benefit from the CO_2-induced water saving effect through stomatal closure, when eCO_2 occurs in combination with periods of water stress. The conserved water enables the C4 plants to extend their growing in dry periods, leading to increased biomass under eCO_2 compared to aCO_2 (Kimball, 2016). The combined effect of transpiration and biomass accumulation can be summarized with the measure water use efficiency (WUE), derived by division of total aboveground biomass by the sum of evapotranspiration. In general, an improvement of WUE of about 10-32% is expected under eCO_2, depending on crop type and water ability (Deryng et al., 2014; O'Leary et al., 2015; Roy et al., 2016).

1.1.2 Experiments for climate impact analysis on crops

Knowledge about effects of eCO_2 on agricultural systems originates from various experiments, in which plants are exposed to increased CO_2 concentrations. Based on more than 70 studies of chamber and greenhouse experiments, Kimball (1992) presented an average increase in crop yield of 33% under doubled CO_2 concentration. However, chamber and greenhouse experiment are discussed to be accompanied with changes in for instance wind speed, air temperature and solar radiation which might lead to different responses of the vegetation compared to field grown crops (Lewin et al., 1994). In order to minimize the

'chamber effect', the free-air carbon dioxide enrichment (FACE) system was developed and applied in 1989 for the first time (Hendrey and Kimball, 1994). FACE facilities consist of a set of vertical vent pipes that emit CO_2 (often depending on the wind direction) to increase the CO_2 concentration within the FACE experiment to a defined level (Lewin et al., 1994) (Figure 1-1). A sensor in the center of the rings measures the CO_2 concentration. The CO_2 fumigation usually runs during daylight hours only and is commonly interrupted when wind speed exceeds 6 m s^{-1} (Kuzyakov et al., 2019). Until today, FACE experiments have been utilized in many different ecosystems around the world covering a wide range of agroecosystems (including grassland), wetlands, deciduous and coniferous forests and a desert (Ainsworth and Long, 2005; Kimball, 2016; Norby and Zak, 2011).

Figure 1-1: Example of a FACE system; Control ring (left) and CO_2-fumigating ring (right) of the FACE experiment on the research field near Giessen, Germany, with C3 grass.

A large number of parameters of the soil-plant system have been measured and investigated using FACE including the effects on aboveground biomass and water fluxes. A mean CO_2-induced decrease in transpiration of 22% was described by Ainsworth and Roger (2007) who conducted a meta-analysis on FACE experimental data. They showed a significant decrease in stomatal conductance for all considered functional groups. Grassland, which covers one third of terrestrial area world-wide, has been studied in a number of grassland FACE experiments (Hovenden et al., 2019, 2014, 2006; Schneider et al., 2004; Suttie et al., 2005). On average, C3 grass is reported to respond to eCO_2 with a decrease in stomatal conductance of more than 30% (Ainsworth and Rogers, 2007). However, the water saving effect through stomatal closure might be counteracted by an increase in aboveground biomass linked with an increase in leaf area index (Manea and Leishman, 2014; Tor-ngern et al., 2015). In general, an average rise in total aboveground

biomass of about 20% for 29 reviewed C3 species grown in FACE experiments, including the largest response with 28% for forests and a smaller response of 10% for C3 grass (475-660 ppm), was shown by Ainsworth and Long (2005). In a long-term FACE experiment on temperate C3 grassland in Giessen, Germany, where CO_2 enrichment was 20% above aCO_2 (Jäger et al., 2003), a significant increase in total aboveground biomass was observed, in particular under average local conditions (Andresen et al., 2018; Kammann et al., 2005; Obermeier et al., 2017). However, the impact on evapotranspiration and WUE of the grassland site has rarely been addressed to for the long-term.

The absence of a CO_2 response of C4 crops under well-watered conditions regarding biomass accumulation was observed in FACE experiments on maize and sorghum (Kimball, 2016). Sorghum (*Sorghum bicolor* L.) was cultivated under an eCO_2 concentration of 561 ppm in Arizona, USA, showing no effect in biomass at final harvest (Ottman et al., 2001). In the FACE experiment in Illinois, USA, maize (*Zea mays* L.) was grown under eCO_2 (550 ppm) resulting in no stimulation of yield, biomass or photosynthesis (Leakey, 2006). In consistence with this, a FACE experiment in Braunschweig, Germany, observed no enhanced biomass production growing maize under eCO_2 of 550 ppm (Manderscheid et al., 2014). However, when eCO_2 was accompanied with periods of drought stress a distinct average increase in harvested biomass of 18% was reported for C4 crops under 550 ppm CO_2 (Kimball, 2016). For instance, Ottman et al. (2001) observed a 15% increase in sorghum biomass at harvest when eCO_2 and water stress were combined. Manderscheid et al. (2014) even reported a substantial biomass increase of 25% at harvest for maize under eCO_2 and water limited conditions. Both studies assume that the crops benefited under FACE during drier periods from saved water as a consequence of stomatal closure. This was confirmed by parallel sap flow measurements in the Braunschweig experiment which resulted in 20% lower transpiration rates under water stress when CO_2 was increased (Manderscheid et al., 2016).

1.1.3 Models for climate change projections on the soil-plant system

Sophisticated environmental experiments such as FACE offer a range of measured soil, plant and atmospheric variables, i.e. they can be perfectly used for model development and testing. Models in turn are important tools for the investigation of CO_2 effects by increasing process understanding, testing for hypothesis or by enabling for projections (Craufurd et al., 2013). The development of agricultural system models dates back to the 1960s (Jones et al., 2017), triggered by the believe in the ability to simulate these systems merging biological and physical principles. Since then, a combination of technological development, food security interests, interdisciplinary collaborations and climate change assessment promoted major advances in agricultural system modelling (Jones et al., 2017). Statistical models have been developed that mainly provide insights into past environmental-plant relationships. Yet the majority is not

well suited for projecting future developments as statistical models cannot reflect changes that are not represented in the monitored data (Lobell and Burke, 2010). Thus, most frequently, process-based models are used to investigate the climate change effect on the soil-plant system (Fodor et al., 2017), where prominent examples are WOFOST, WOrld FOod STudies (Diepen et al., 1989), APSIM, Agricultural Production Systems Simulator (Keating et al., 2003), and EPIC, Erosion-Productivity Impact Calculator (Williams et al., 1989).

In a number of modelling studies, the impact of eCO_2 on transpiration, soil moisture and plant growth has been simulated (Betts et al., 2007; Cheng et al., 2014a; De Kauwe et al., 2013; Gedney et al., 2006; Jin et al., 2018; Zaehle et al., 2014). Tubiello et al. (2007) find, that most crop model results are in line with FACE experimental observations. However, recent multi-model investigations, related to the Agricultural Model Inter-Comparison and Improvement Project (AgMIP), described the need for a better representation of biomass and water balance processes, as well as an improved representation of CO_2 responses in C4 and C3 crops such as maize and grassland systems (Bassu et al., 2014; Durand et al., 2017; Ruane et al., 2017; Sándor et al., 2016a, 2016b). For instance, a study by Durand et al. (2017) revealed clear limitations in simulating maize biomass under eCO_2 and drought stress, applying 21 established maize models to the maize-based FACE dataset of Braunschweig, Germany. To move forward, accurate response functions that simulate the effect of eCO_2 on biomass production and stomatal opening are needed and should be calibrated with recent FACE data. Morison (1987) reported a linear increase in stomatal resistance based on a literature analysis of 23 C3 and C4 studies. He further described a 40% rise in stomatal resistance when CO_2 increased from 330 ppm to 660 ppm. These observations were implemented in the EPIC model and represented as a simple CO_2 response function including the stomatal response factor $p = 0.4$, to consider the 40% increase in stomatal closure (Stöckle, 1992). This was observed before the first FACE experiment was conducted. Later, Wand et al. (1999) updated values for the factor p based on open-top chamber and FACE experiments, e.g. $p = 0.24$ for C3 grasses and $p = 0.29$ for C4 grasses. A simple approach for simulating the impact of eCO_2 on net assimilation was presented by Goudrian et al. (1984). Soltani and Siclair (2012) adapted this approach to simulate the effect of eCO_2 on the radiation use efficiency using the response factor b, where $b = 0.8$ for C3 and $b = 0.4$ for C4 plants. However, both CO_2 response factors have not been updated using FACE data of maize or grassland.

Recent model development suggest to use flexible programming environments to set up user-adapted models, instead of adding more and more routines into one model code (Clark et al., 2011). Further, regarding the simulation of hydrological processes, Eitzinger et al. (2004) recommended the use of multiple layer approach models after comparing three established crop models with different complexity of soil water models in their study, indicating that variation in soil water content is one of the major reasons for variations in simulated biomass. In line with this, this work is based on coupling a plant growth model with a

hydrological model. The Catchment Modelling Framework (CMF) and the Plant Growth Modelling Framework (PMF) are integrative and flexible tools that facilitate customized model setups specifically adapted to a given research question (Houska et al., 2014; Kraft et al., 2011; Multsch et al., 2011). An uncertainty analysis is essential before any modelling exercise (Pappenberger and Beven, 2006). In crop modelling, recent studies revealed distinct uncertainties, which have rarely been addressed to before (Rötter et al., 2011; Vanuytrecht and Thorburn, 2017). The coupled model used in this study comes along with a number of parameters. In order to avoid overfitting and to analyse parameter uncertainty, a sensitivity analysis was conducted, followed by an uncertainty analysis similar to the GLUE approach proposed by Beven and Binley (1992). The Monte Carlo based approach follows the concept of equifinality, i.e. different parameter sets can produce equally good results. Using Latin Hypercube sampling a number of parameter sets was created. Parameter sets that led to acceptable and so called 'behavioral' model runs were selected based on pre-defined criteria. Parameter sets which resulted in model runs that did not fulfil the pre-defined criteria were non-behavioral and therefor rejected, i.e. deleted.

1.1.4 Objectives

The aim of this dissertation was to couple a hydrological and a plant growth model for the investigation of climate change effects on agricultural systems. In detail, this work aimed at developing and testing a tool that is capable to accurately simulate the CO_2 effect on biomass and water fluxes for both C3 and C4 plants. For this, two objectives were defined, which have been tackled in two accepted publications:

1) Set up a process-based coupled hydrological-plant growth model to simulate effects of elevated atmospheric CO_2 on the soil-plant system.

The first objective was accomplished by coupling the hydrological model CMF with the plant growth model PMF. In order to enable the investigation of eCO_2 on the soil-plant system, PMF was further developed in this work with an evapotranspiration model for sparse crops and straightforward CO_2 response functions. For robust parametrization, a sensitivity test was conducted, followed by a parameter uncertainty analysis applying a rejectionist Monte Carlo approach and following the concept of equifinality. Applying the model to data of a long-term C3 grassland FACE experiment in Giessen, Germany, effects of eCO_2 on biomass and water dynamics were investigated (Chapter 2).

2) Investigate the model's suitability to project the combined effect of eCO_2 and drought stress on the C4 crop maize.

In order to achieve the second objective, the coupled hydrological-plant growth model CMF-PMF was applied to data of the two year FACE experiment in Braunschweig, Germany, where the C4 crop maize was

fumigated with CO_2 under wet and a dry conditions in 2007 and 2008. The model was calibrated under wet conditions under aCO_2 and eCO_2 in 2007 including CO_2 response parameters applying again the rejectionist Monte Carlo approach. Then, the model was successfully validated and the effect of eCO_2 and drought on biomass and water fluxes was investigated (Chapter 3).

1.2 Material and Methods

1.2.1 Study sites and data

1.2.1.1 Grassland FACE experiment (C3)

For the simulation of the CO_2 effect on C3 grassland (objective 1), long-term data (1999-2011) of a FACE experiment near Giessen, Hesse, Germany (50°32'N and 8°41'E, 172 m above sea level) was used (Figure 1-2). The still ongoing experiment started in 1998, including three ambient rings and three elevated rings with a 20%-increased CO_2 concentration (Jäger et al., 2003). The vegetation type is tall oat-grass (*Arrhenatheretum elatioris – Filipendula ulmaria* sub-community, Kammann et al. (2005)), where C3 grasses accounted for 73% of the total aboveground biomass, followed by forbes with 24% and legumes with 3%. The non-ploughed, temperate grassland was fertilized with 40 kg N ha^{-1} $year^{-1}$. The soil is a *Fluvic Gleysol* and the soil type is a sandy clay loam with a soil porosity between 60 and 65%.

As model input data, groundwater measurement data on weekdays and meteorological data was used which is measured on the study site, including daily values of minimum and maximum temperature, wind speed, solar radiation, sum of precipitation and relative humidity. Between 1999 and 2011 the study site was characterized with a mean annual precipitation of 573 mm and a mean annual temperature of 9.8°C. The CO_2 concentration was on average 394 ppm in the ambient rings, and 483 ppm in the elevated rings between 1999 and 2011.

For model calibration, total aboveground dry matter and soil moisture between 1999 and 2011 was used. The grassland was harvested twice a year (Table S 2-2), showing on average higher yields at the first harvest compared to second harvest. Soil moisture data was available on several days per week measured in 0.15 m depth. On average the soil moisture content was 37.0% in the ambient rings and 38.4% in the elevated rings.

1.2.1.2 Maize FACE experiment (C4)

For the simulation of the combined effect of eCO_2 and drought stress on the C4 crop maize (objective 2), data of a FACE experiment with *Zea mays* L. in Braunschweig, Germany (52°18'N and 10°26'E, 79 m above sea level) was used (Figure 1-2). The experiment was conducted in the years 2007 and 2008, including three ambient rings with 378 ppm and three elevated rings with 550 ppm CO_2 (Manderscheid et al., 2014). The CO_2-fumigation started in June, when the leaf area index reached 0.5 m^2 m^{-2}. The maize was fertilized with

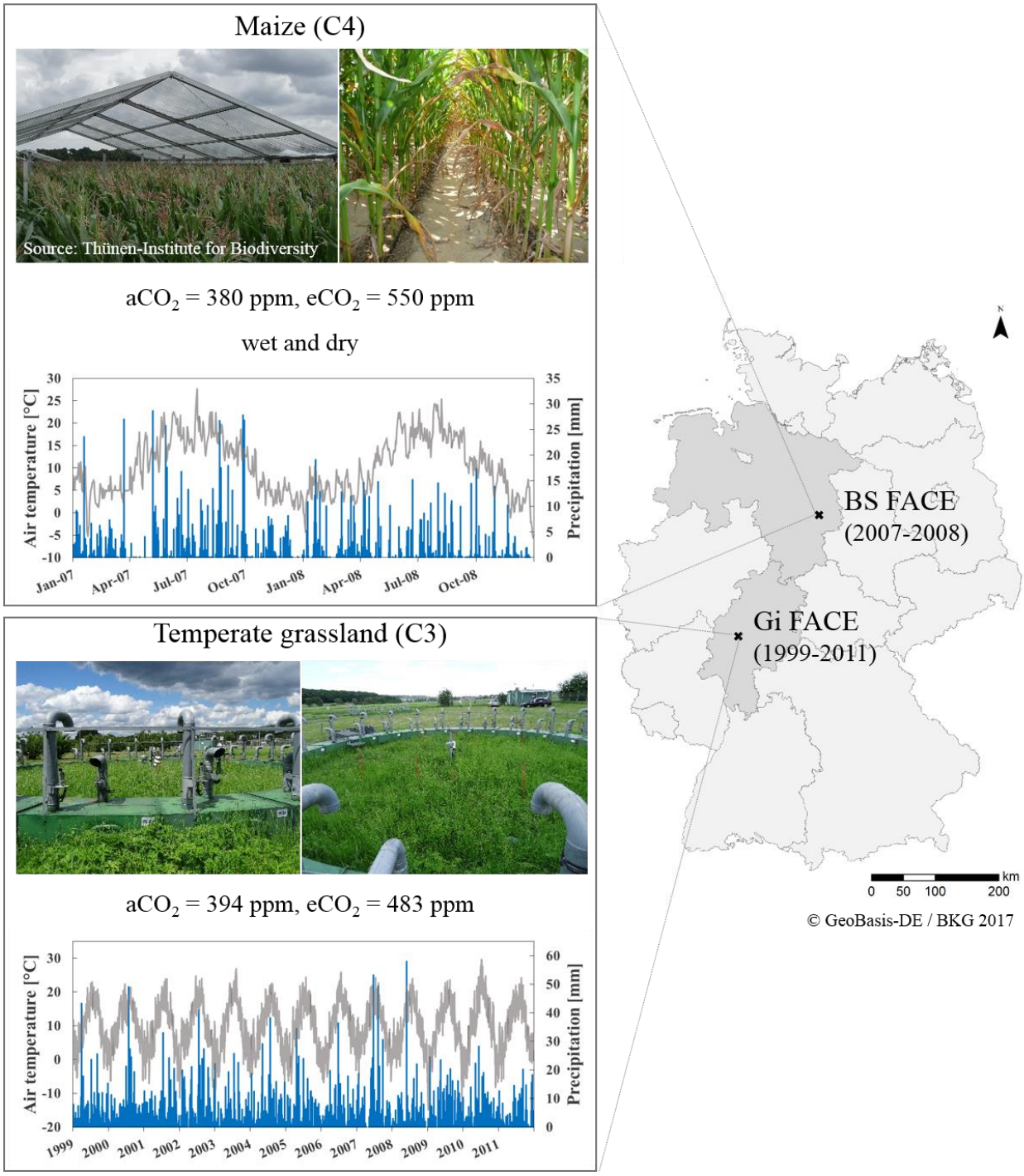

Figure 1-2: Overview of the two study sites used in this study, including the Giessen FACE experiment (GiFACE) in Hesse, Germany with temperate C3 grassland and the Braunschweig FACE experiment (BS FACE) in Lower-Saxony, Germany, with maize (C4).

180 kg ha^{-1} mineral nitrogen fertilizer and was further managed according to standard farm practices. The soil was a loamy sand texture followed by a mixture of gravel and sand in deeper soil layers. In order to investigate the combined effect of eCO_2 and drought stress, one half of each ring was well-watered (wet) whereas the other half was water limited (dry).

As forcing data, meteorological data was given. The considered parameters sum of precipitation, wind speed, solar radiation, minimum and maximum temperature and relative humidity were measured on the study site. The mean temperature was 10.4°C in the year 2007 and 10.3°C in 2008. Precipitation in combination with irrigation resulted in 878 mm and 715 mm in the wet treatment in the two consecutive years. The water input was reduced to 835 mm and 552 in the dry treatment in the years 2007 and 2008 by excluding precipitation water with for instance rain shelters in 2008. 2007 was an exceptional wet year, resulting in a reduction of water input of only 43 mm compared to a reduction of 163 mm in 2008.

For model evaluation, total aboveground biomass and soil moisture were taken. The biomass was measured three to four times per growing season. The soil water content was measured twice a week and in three different depths using portable TDR sensors (Manderscheid et al., 2014).

1.2.2 The coupled hydrological-plant growth model

Various model types are applied for the investigation of climate change impacts on agricultural system, most frequently these are process-based crop models (Fodor et al., 2017). In this work, the process-based coupled hydrological-plant growth model CMF-PMF was used to investigate climate change effects on the complex soil-plant system. The coupled model, including the further development of PMF with CO_2 response functions, is also described in detail in chapter 2.

1.2.2.1 The hydrological model (CMF)

The Catchment Modelling Framework (CMF), developed by Kraft et al. (2011), is an open-source programming library (Kraft et al. (2018), https://github.com/philippkraft/cmf) which can be used to create modular, process-based hydrological models. The core classes and functions are written in C++. However, CMF can easily be coupled with other models using the Python programming language as an interface. CMF can be used for one- to three-dimensional representation of a hydrological system (Djabelkhir et al., 2017; Houska et al., 2017; Maier et al., 2017; Windhorst et al., 2014). In this work, CMF was used to create a 1D plot model, including a site specific number of soil layers. Water fluxes between the layers were calculated with a daily time step according to the Richards‘ equation (Richards, 1931) and soil hydraulic properties were defined using the van Genuchten-Mualem function (van Genuchten, 1980), considering site specific

soil parameters for saturated conductivity (k_{sat}), porosity (φ), pore size distribution (n) and the inverse of water entry potential (α).

1.2.2.2 The plant growth model (PMF)

The Plant growth Modelling Framework (PMF), developed by Multsch et al. (2011), is a modular, generic tool, which can be used to set up customized crop models. The framework is implemented in Python and available as free software (www.github.com/jlu-ilr-hydro/pmf). Similar to CMF, PMF is easily expandable and connectable to other models. PMF is composed of four core elements: *Plant Model*, *Process Library*, *Crop Database* and *Plant Building Set*. The *Plant Model* creates the connection of the structural organs and the related growth processes. The *Process Library* contains a set of independent classes defining next to others plant development and uptake of water. The *Crop Database* provides relevant crop specific parameters and the *Plant Building Set* connects the three core modules. Plant development is simulated applying the thermal time concept (Monteith and Moss, 1977), i.e. the plant passes various development stages according to a temperature sum. The temperature sum is obtained by accumulation of so-called growing degree days (GDD, [°days]) using $GDD = (t_{max} + t_{min})/2 - t_{base}$ with the daily maximum temperature t_{max} [°C], the daily minimum temperature t_{min} [°C] and the base temperature t_{base} [°C] which serves as a threshold below which no plant development occurs. Biomass accumulation is simulated with a daily time step applying the radiation use efficiency concept (Monteith and Moss, 1977), where photosynthetically active radiation is transformed into total dry biomass using the radiation use efficiency factor (rue). Produced biomass is then distributed to different aboveground (leaves, stem and storage organ) and belowground (roots) plant organs depending on the development stage. A response to water stress is considered in PMF based on Feddes et al. (1978), where a water stress factor, which is derived by the ratio of actual and potential transpiration, hampers biomass accumulation.

1.2.2.3 Further development of PMF

In order to enable the investigation of climate change effects on agricultural systems, the plant growth model PMF was further developed. In a first step, the sophisticated evapotranspiration model according to Shuttleworth-Wallace (SW) was implemented (Shuttleworth and Wallace, 1985). In a second step, CO_2 response functions to stomata and biomass accumulation were added (Figure 1-3).

The SW approach calculates evapotranspiration from soil and vegetation as two different sources, including a network of five coupled resistances, e.g. soil surface resistance (r_s^s), aerodynamic resistance from soil to canopy (r_a^s), aerodynamic resistance from canopy to reference height (r_a^a), bulk boundary layer resistance of canopy (r_a^c) and the bulk stomatal resistance of the canopy (r_s^c), all resistances in [s m^{-1}] (Hu et al., 2009; Shuttleworth and Wallace, 1985). In this study, r_s^c was affected by the effective leaf area index as well as by a product of three environmental stress functions that controlled stomatal response to a change in vapor

pressure deficit (vpd_{res}), temperature ($temp_{res}$) and atmospheric CO_2 (co_{2res}). The simple response functions to air temperature and vapor pressure deficit where implemented according to Zhou et al. (2006), whereas as the CO_2 response function was taken according to Stöckle et al. (1992). All three stomatal response functions return a value between 0 and 1, where 0 implies closed stomata and 1 means stomata are opened to the maximum. vpd_{res} calculates an increasing stomatal closure, when the vapor pressure deficit is rising. This is counteracted by the simulated $temp_{res}$, which describes an increase in stomatal opening from 0 (when the air temperature is below 0°C) to 1 (when the air temperature is above 25°C). co_{2res} leads to stomatal closure, when the measured CO_2 concentration increases (Figure 1-4a). The extent of this response is controlled by the plant-specific factor *p*. The larger the response parameter *p*, the stronger is the effect on the closure of the stomata. For an accurate estimation of the CO_2 effect on stomatal opening, this factor needs to be parametrized using FACE data.

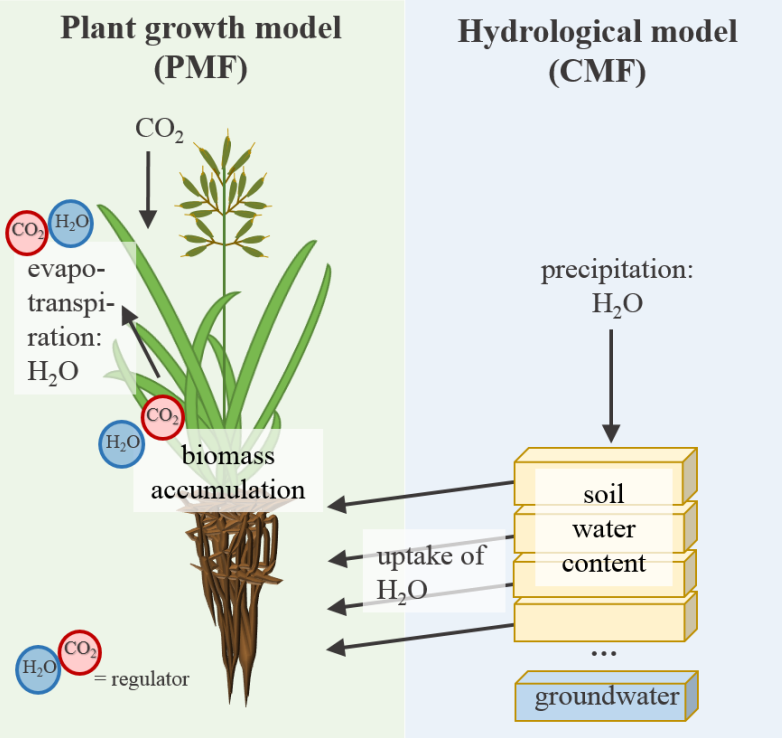

Figure 1-3: Simplified representation of the coupled hydrological-plant growth model setup CMF-PMF as used for the Giessen study site, including water fluxes and CO_2 responses.

In addition to the SW approach including the stomatal response functions, a response function for the radiation use efficiency (rue_{CO2}) was implemented after Soltani and Sinclair (2012). Here, rising measured CO_2 concentrations (co_{2meas} [ppm]), which exceed a reference CO_2 concentration (co_{2ref} [ppm]), result in an

improved radiation use efficiency. This effect is amplified by an increase in a factor *b*, e.g. the larger factor *b*, the stronger is the increase in rue_{CO2} and, in turn, the biomass accumulation (Figure 1-4b). Similar to factor *p*, factor *b* needs to be parametrized using FACE data, in order to achieve an accurate simulation of the CO_2 effect on biomass accumulation.

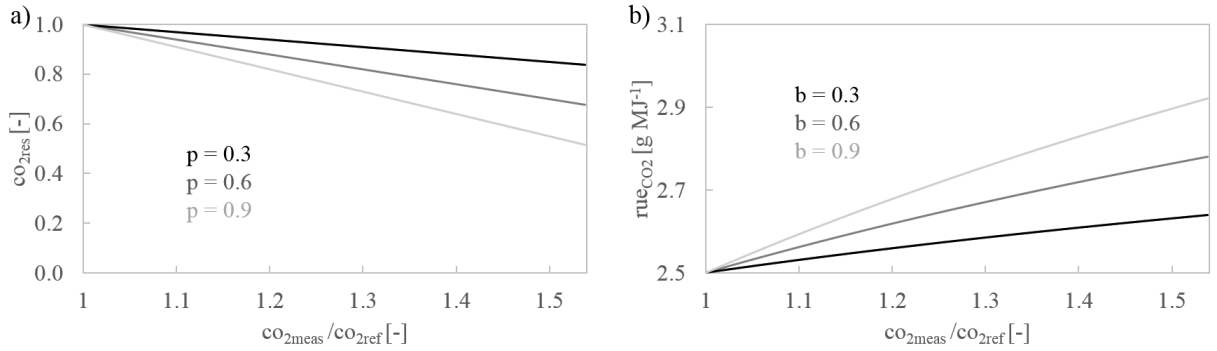

Figure 1-4: CO_2 responses as implemented in PMF. Depending on the ratio of the measured (co_{meas}) and the reference CO_2 concentration (co_{2ref}), a) shows the CO_2 response of the stomata (co_{2res}) for different values of the response factor *p*, and *b*) shows the CO_2 response of the radiation use efficiency (rue_{CO2}) for different values of the response factor *b* when the reference rue is set to 2.5 g MJ^{-1}.

1.2.2.4 Coupled CMF-PMF

As recommended for scientific research by Perkel (2015), the Python programming language was used to couple the hydrological and the plant growth model. Considering the states of CMF at time step *t*-1, PMF simulates the evapotranspiration and biomass accumulation including development of the leaf area index at time step *t*. Thereafter, CMF proceeds taking into account the calculated plant water demand and the changes in interception capacity as a result of leaf area development.

1.2.3 Sensitivity and uncertainty analysis

In order to identify the most sensitive parameters, a Fourier amplitude sensitivity test (FAST) was established according to Saltelli et al. (1999). Applying the FAST method, the total contribution of every input parameter to the output's variance can be calculated. The SPOTPY open-source python package developed by Houska et al. (2015) was used to run the sensitivity analysis on eighteen input parameters, including fourteen plant specific (PMF) parameters and four hydrological (CMF) parameters. A required minimum number of 39,000 model runs was estimated to fulfil the FAST algorithm's criteria (Henkel et al., 2012). A detailed description of the conducted analysis is available in the Supporting Information Figure S 2-1.

In order to analyse the parameter uncertainty, a rejectionist Monte Carlo approach was conducted (Beven and Binley, 1992) using SPOTPY. The method followed the concept of equifinality, i.e. instead of calibrating the coupled model to a single optimum parameter set, a collection of different parameter sets that produce equally good results, was analysed. Usually, the parameter sampling is executed using the Monte Carlo algorithm. To improve the sampling and in view of the large number of parameters to be calibrated, a Latin Hypercube (LH) sampling approach was applied according to McKay et al. (1979). Firstly, a potential range for each parameter was defined based on expert knowledge and literature values. Then, a number of parameter sets was picked by the LH sampling method, assuming a uniform distribution, and the model was run with each of the parameter sets. Finally, the behavioural runs were determined comparing simulated with measured data. In this work, the target values were biomass and soil moisture. Using objective functions, e.g. the root-mean-squared-error (RMSE), the coefficient of determination (r^2) or the bias, acceptance criteria were defined and only those simulations that fulfilled the criteria were considered in the further analysis. The final selection of the objective functions is depending on the research question and has to be selected accordingly. In our studies, the rejectionist Monte Carlo method was applied iteratively in order to optimize the simulations and to increase the number of final parameter sets, i.e. based on the results of previous set of model run the parameter ranges were adapted and again, new parameter sets were created.

1.3 Results and Discussion

1.3.1 Simulating the effect of CO_2 on grassland (C3)

Grasslands cover one third of the global terrestrial area (Suttie et al., 2005) and represent an important ecosystem that has been rarely investigated regarding CO_2 effects on water fluxes. The results of the simulated CO_2 effect on a C3 grassland, including a sensitivity and uncertainty analysis of the coupled hydrological-plant growth model are described in detail in chapter 2 and are published in the publication:

Kellner, J., Multsch, S., Houska, T., Kraft, P., Müller, C., Breuer, L., 2017. A coupled hydrological-plant growth model for simulating the effect of elevated CO_2 on a temperate grassland. Agricultural and Forest Meteorology 246, 42–50. https://doi.org/10.1016/j.agrformet.2017.05.017

1.3.1.1 Sensitivity and uncertainty analysis and model performance

Applying the FAST approach to the coupled hydrological-plant growth model, the number of prior eighteen parameters was reduced to eleven sensitive parameters, including three hydrological parameters and eight plant specific parameters (Supporting Information Table S 2-3). The uncertainty analysis revealed an

uncertainty range of 5% in soil moisture and 19 g dry matter m^{-2} in biomass related to the eleven parameters. The CO_2 response parameter for biomass accumulation, factor *b*, ranged between 0.1-0.3 for the long-term FACE experiment with temperate C3 grassland in Giessen, which was lower than the value of 0.8 suggested by Soltani and Sinclair (2012). The stomatal response parameter, factor *p*, showed at peak at 0.3, which was in line with results of Wu et al. (2012) who reported $p = 0.24$ for pastures with C3 grass. The performance of the coupled model was good in simulating biomass with an r^2 of 0.3-0.6, a bias of 0-80 g dry matter m^{-2} and an RMSE of 122-155 g dry matter m^{-2}. For example, Sándor et al. (2016b) reported $r^2 < 0.3$ when simulation grassland biomass with a model ensemble, though Moot et al. (2015) resulted in a smaller RMSE of 65 g dry matter m^{-2} when calibrating the APSIM model for lucerne. The pattern of measured higher yields at first harvest and lower yields at second harvest was well presented by the model (Figure 2-1a-e), but limitations in a harvest-wise analysis appeared comparing simulated increase in biomass (9% and 2%) at first and second harvest with measured data (6% and 13%). The course of higher soil moisture values in winter and lower soil moisture values in summer was well mapped by the coupled model (Figure 2-1f-j), with an r^2 of 0.4 to 0.7 vol.%, a bias of -7 to 0 vol.%. and an RMSE of 6 to 10 vol.%. The accurate representation of soil water processes has been described as a challenge in grassland ecosystem modelling resulting in an r^2 of 0.1-0.7 (Sándor et al., 2016b, 2016a). In periods when the soil was close to saturation according to the measured data, the coupled model underestimated the measured soil moisture. Different sources, e.g. limitation of the van Genuchten-Mualem analytical function (Schaap and Van Genuchten, 2006), simplified consideration of soil parameters for the soil column, but also possibly larger errors in the monitoring data under almost saturated conditions (IMKO Micromodultechnik GmbH, 2001), might have contributed to this results.

1.3.1.2 eCO_2 effect on biomass, soil moisture and water fluxes

A significant increase in the harvested grassland biomass by +6.5% was simulated under eCO_2. This was in line with a measured increase in biomass of +9.1%. The results were in agreement with findings of Ainsworth and Long (2005), who reported an average gain in grassland biomass of +10% analyzing FACE studies with 475-600 ppm eCO_2. Soil moisture content was not affected by eCO_2 in the temperate grassland of the Giessen FACE. Likewise, the evapotranspiration remained the same, i.e. no significant increase was simulated. However, dividing evapotranspiration into evaporation and transpiration showed a decline in evaporation of -1.4% and a rise in transpiration of +0.8% (Figure 1-5a). A similar effect was reported for expanded grassland by Liu et al (2009) showing increased transpiration but decreased evaporation as a result of reduced soil evaporation. The enhancement of transpiration under eCO_2 showed that water savings at leaf level, induced by closed stomata, were counteracted at stand level by an increased leaf area index. An offset of the stomatal effect in a temperate grassland due to an increased leaf area index under eCO_2 was also shown by Manea and Leishman (2014). The water use efficiency, i.e. the ratio of annually harvested biomass

and accumulated evapotranspiration from March to September, was simulated to increase by +5.4% under eCO_2 at the grassland research area in Giessen. Considering the moderate eCO_2 fumigation level of 483 ppm, the relatively small, though significant increase, is in line with a reported global raise of crop water use of 10-27% under 550 ppm (Deryng et al., 2016) or a 30% increase in water use efficiency of wheat under 550 ppm (O'Leary et al., 2015). In summary, the findings of this study indicate that temperate, mown, wet-dry C3 grassland might benefit from biomass increase while retaining water consumption, i.e. evapotranspiration, already when CO_2 concentration is enhanced by 20% compared to aCO_2. Further, the expected water saving at a leaf level can be offset at a stand level as a result of increased transpiration, caused by a biomass gain under a 20% increase of CO_2.

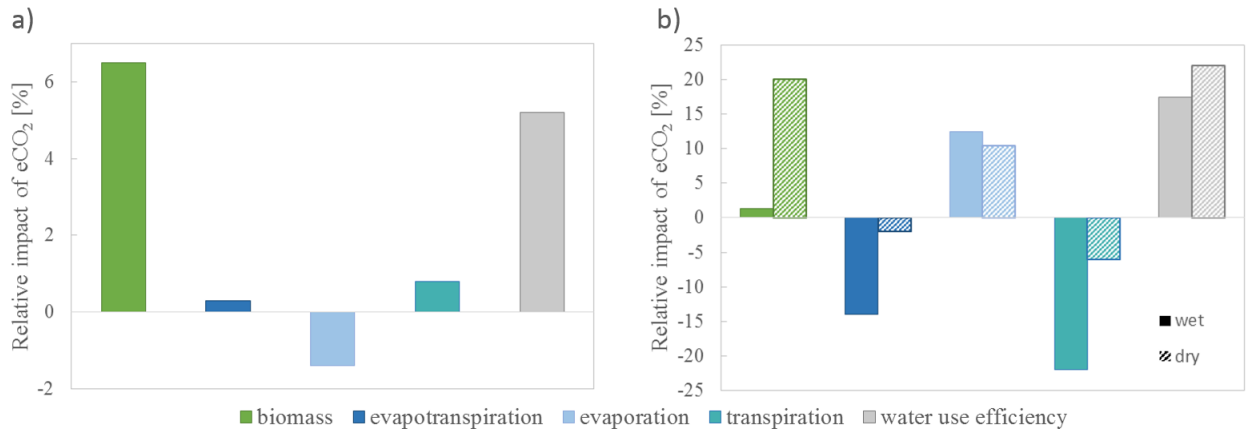

Figure 1-5: Simulated relative impact of eCO_2 on biomass, water fluxes (evapotranspiration, evaporation, transpiration) and water use efficiency [%]; a) temperate grassland (C3) in Giessen, Germany with 20% increased CO_2 for the years 1999-2011; b) maize (C4) in Braunschweig, Germany with aCO_2 = 380 and eCO_2 = 550 ppm in 2008 under wet and dry conditions (note the differences of the y–axis scale in both panels).

1.3.2 Simulating the combined effect of eCO_2 and drought on maize (C4)

A recent study by Durand et al. (2017) revealed strong limitations in simulating the combined effect of eCO_2 and drought on maize using an ensemble of 21 established maize models. In this work, the coupled hydrological-plant growth model was applied to the same maize FACE data, including a calibration of CO_2 response factors *b* and *p*. The results of the uncertainty analysis and the model validation as well as the simulated combined effect of eCO_2 and drought are described in detail in chapter 3 and are summarized in the publication:

Kellner, J., Houska, T., Manderscheid, R., Weigel, H.-J., Breuer, L., Kraft, P., 2019. Response of maize biomass and soil water fluxes on elevated CO_2 and drought – from field experiments to process-based simulations. Global Change Biology 25, 2947-2957. https://doi.org/10.1111/gcb.14723

1.3.2.1 Model calibration, validation and uncertainty analysis

In this study, the two-years data set of the maize FACE experiment in Braunschweig, Germany, was splitted in order to calibrate the coupled model with biomass and soil moisture data of 2007 and to validate the model with data of 2008, where eCO_2 was combined with distinctly reduced water input, leading to drought stress in 2008. The calibrated CO_2 response parameter *b* for biomass accumulation resulted in very small values of <0.1 for the C4 plant maize based on data of FACE experiment in Braunschweig. Hereby, the biomass response to eCO_2 was smaller than suggested by Goudriaan et al. (1984) for C4 plants (b = 0.4). The stomatal CO_2 response parameter *p* showed values >0.7. This was above the value of p = 0.4 given by Stöckle et al. (1992) and the value of 0.29 adapted by Wand et al. (1999) for C4 pastures. In the calibration year 2007, model performance was very good in terms of biomass simulation with an RMSE of 1.3 Mg ha^{-1} (Figure 3-2). In the validation year 2008, the RMSE was slightly higher, with an RMSE of about 1.7 Mg ha^{-1} and 2.4 Mg ha^{-1} in the wet and dry treatment, respectively. Compared to other publications, this performance was very good. For example, Cavero et al. (2000) described an RMSE of 3.8 Mg ha^{-1} applying the EPIC model for simulating maize under water-limited conditions in Spain. Durand et al. (2017) reported an RMSE of 2.1 Mg ha^{-1} applying an ensemble of 21 established maize models to the Braunschweig FACE data in 2007 and 2008. The performance of the coupled model regarding soil moisture was also very good with an RMSE of <6% in 2007 and <7% in 2008. A similar RMSE between 5-9% was calculated by Saseedran et al. (2005), who compared soil moisture measurement of different maize hybrids in the US to simulations with the CEREZ-Maize model.

1.3.2.2 Combined effect of eCO_2 and drought on biomass, soil moisture and water fluxes

In both years, CO_2 enrichment to 550 ppm was combined with a wet and dry treatment. In 2007, the reduction of water input was very small (<50 mm), leading to no simulated water stress in the dry rings in 2007. In both treatments in 2007 and in the wet treatment in 2008, the CO_2 enrichment resulted in no relevant simulated biomass gain, which was in line with the measured biomass data. Further, there was no increase in soil moisture simulated, which was in consistence with the observed data (Manderscheid et al., 2014). However, in the dry treatment in 2008, the coupled model simulated a significant CO_2-induced increase in harvested biomass of +20% (Figure 1-5b). A distinct biomass gain was also observed in the field, showing an increase of 25%. The absence of a CO_2 effect on biomass for the C4 crop maize in 2007 and in the wet treatment in 2008 could only be simulated with a very small CO_2 response factor *b*, approving the small size of the factor. The masked increase of 20% in the dry treatment in 2008, was a result of the relative high stomatal CO_2 response factor *p*. Values of $p > 0.7$ reduced water losses by reducing transpiration under

eCO_2, i.e. water stress was significantly diminished and hence, the plant could continue producing biomass in periods of water-limited conditions. In line with Durand et al. (2017), this study shows that an explicit stomatal response is needed to enable the simulation of a strong CO_2 response under water limited conditions and to project a reduction in water stress.

In 2007 and in the wet treatment in 2008, transpiration was reduced by -22% under eCO_2, which is in agreement with Manderscheid et al. (2016), who observed a decrease of transpiration by -20% conducting sap flow measurements in the maize FACE experiment in 2007 and 2008 in Braunschweig. Further, a significant CO_2-induced reduction of transpiration in the C4 crop maize was reported by Hussain et al. (2013), who analysed maize grown in a FACE experiment in the US under 550-585 ppm eCO_2. The simulated reduction of transpiration, as a result of the high values of the stomatal response factor *p*, in turn contributed to a simulated increase in evaporation (+8-12.5%) and an overall reduction in total water consumption, i.e. evapotranspiration, in 2007 (-15%) and the wet treatment in 2008 (-14%). However, in the dry treatment in 2008, the simulated reduction in transpiration was small (-6%) under eCO_2 (Figure 1-5b). This was in line with the reported sap flow measurements that resulted in even no reduction under eCO_2 (Manderscheid et al., 2016). The evapotranspiration was also only reduced by -2% under eCO_2. This small overall reduction shows, that the water saving effect on a leaf level, was counteracted on a stand level by the 20% biomass increase, and hence leaf area increase. In summary, in this study, the clear benefit of the C4 plant maize from eCO_2 under water-limited conditions was successfully simulated, including improved results compared to biomass simulations of a model ensemble with 21 maize models reported by Durand et al. (2017). The validation of the coupled hydrological-plant growth model was successful, although the environmental conditions were distinctly different during the calibration period. This proves the assumption that the coupled model covers the relevant climate change feedback mechanisms on plant growth. The obtained values of the calibrated response parameters can be used in other crop models to project maize yields under climate change conditions.

1.4 Conclusion and Outlook

In this work, a robust tool for the investigation of climate change effects on C3 and C4 plants was established, by further developing, calibrating and validating a coupled hydrological-plant growth model with up-to-date FACE experimental data. In two steps, a process-based coupled model was set up to simulate effects of eCO_2 on the soil-plant system and then, the model's suitability to project the combined effect of eCO_2 and drought stress on the C4 crop maize was rigorously tested. Based on the experience gained in this work, a simple blueprint with recommendations regarding a comprehensive crop modelling method (i.e. selection of model structure, model optimization strategy, required experimental data) can be deduced.

Selection of model structure – Use a flexible tool! A flexible programming environment to set up customized process-based models is recommended, instead of inserting an increasing number of routines into one model code (Clark et al., 2011). In line with this, model frameworks such as CMF and PMF enable to set up models adapted to a specific research question and study site providing a simple way to add, select or deselect mechanisms. Using CMF, soil properties can be set according to available site specific information, such as depth of soil moisture and porosity measurements. The generic structure of PMF broadens the potential scope of application, e.g. various crop types, such as C3 and C4 plant species.

Model optimization strategy – Do an uncertainty analysis! In order to obtain a robust tool for climate change projections on the plant-soil system, an uncertainty analysis of the model is needed (Pappenberger and Beven, 2006; Rötter et al., 2011). Until a few years ago, little has been done to assess the uncertainty of crop models (Jones et al., 2017). Parameter uncertainty, which shows to what extend the considered parameters contribute to the model output uncertainty can be analysed conducting a rejectionist Monte Carlo analysis as shown in this work. Other sources of uncertainty, i.e. input data and model structure, which were not investigated in this study, might need increased attention in future research. Even though, Nendel et al. (2009) tested the model structure regarding six different CO_2 response algorithms and showed that they caused only minor differences in model performance. However, the need for improved model structures, i.e. more accurate representation of biomass production, soil temperature and soil water to reduce uncertainty, is illustrated by multi-model intercomparison projects for grassland models (Houska et al., 2017; Ma et al., 2014; Sándor et al., 2016b, 2016a) and by a large number of intercomparison studies on wheat (Asseng et al., 2014; Kollas et al., 2015; Rosenzweig et al., 2014, 2013; Rötter et al., 2012). In addition, the use of benchmark data sets for plant growth models as reported by Asseng et al. (2015) is helpful to identify uncertainties.

Required experimental data – Utilize FACE data for model calibration and validation! The methodology presented in this work is based on the use of available FACE data. A large number of parameters of different agricultural systems under free air conditions and eCO_2 can be derived using FACE. Comprehensive datasets that provide soil moisture and biomass data and that include single effects (eCO_2) and combined effects (eCO_2 and drought) enable for a rigorous assessment of crop models and their applicability to project yields and water fluxes under climate change. To improve the simulations of eCO_2 effects on crops, straightforward CO_2 response mechanisms are suitable, but the relevant response parameter which originate from greenhouse and chamber experiments need to be updated with free air experimental data obtained with FACE studies. Thus, this work showed that the increase in radiation efficiency due to elevated CO_2 is important for modelling the CO_2 response of temperate C3 grassland, but should and can be excluded for the C4 plant maize. Finally, we should intensify and improve collaboration of experimentalists and modelers

(Seibert and McDonnell, 2002) in order to collect valuable data to improve the models that are used to project climate change effects on agricultural systems.

In future studies, the coupled hydrological-plant growth model can serve for the investigation of further climate change effects on agricultural systems, for instance regarding temperature or progressive nitrogen limitation considering a number of various crops. In PMF, a stomatal response mechanism to varying air temperature is already implemented. Applying the model to FACE experimental data, where eCO_2 is combined with increased air temperature the coupled model can be calibrated and validated. Subsequently, the coupled effect of increased temperature and eCO_2 could be investigated and, running the model with climate projection data, also effects of different climate scenarios could be analysed. Increased CO_2 may result in less available nitrogen, which is described as a progressive nitrogen limitation (Luo et al., 2006). In PMF, nitrogen demand and uptake can be calculated. Further, a nitrogen stress function is available, which reduces biomass production if nitrogen demand cannot be covered. To start with, information of the available nitrogen content in soil could be obtained by coupling the coupled CMF-PMF with a simplified nitrogen module, e.g. the decomposition model DECOMP (Wallman et al., 2006) could be included as previously shown by Kraft et al. (2010). The model should then be applied to FACE data, where coupled effect of eCO_2 and different nitrogen fertilization levels are investigated. Finally, the coupled hydrological-plant growth model can contribute to investigation CO_2 effects especially on water fluxes in the soil-plant system, e.g. expensive experimental studies can be enhanced by simulating evapotranspiration, evaporation and transpiration. Further, process-based models like the coupled CMF-PMF can be used to test hypotheses, e.g. regarding the progressive nitrogen limitation.

2 A coupled hydrological-plant growth model for simulating the effect of elevated CO_2 on temperate grassland

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Abstract

Elevated CO_2 (eCO_2) reduces transpiration at the leaf level by inducing stomatal closure. However, this water saving effect might be offset at the canopy level by increased leaf area as a consequence of eCO_2 fertilization. To investigate this bi-directional effect, we coupled a plant growth and a soil hydrological model. The model performance and the uncertainty in model parameters were checked using a 13 year data set of a free-air carbon dioxide enrichment (FACE) experiment on grassland in Germany. We found a good agreement of simulated and observed data for soil moisture and total above-ground dry biomass (TAB) under ambient CO_2 (~395 ppm) and eCO_2 (~480 ppm). Optima for soil and plant growth model parameters were identified, which can be used in future studies. Our study presents a robust modelling approach for the investigation of effects of eCO_2 on grassland biomass and water dynamics. We show an offset of the stomatal water saving effect at the canopy level because of a significant increase in TAB (6.5%, $p < 0.001$) leading to an increase in transpiration by +3.0 ±6.0 mm, though insignificant ($p = 0.1$). However, the increased water loss through transpiration was counteracted by a significant decrease in soil evaporation (-2.1 ±1.7 mm, $p < 0.01$) as a consequence of higher TAB. Hence, evapotranspiration was not affected by the increased eCO_2 (+0.9 ±4.9 mm, $p = 0.5$). This in turn led to a significantly better performance of the water use efficiency by 5.2% ($p < 0.001$). Our results indicate that mown, temperate grasslands can benefit from an increasing biomass production while maintaining water consumption at the +20% increase of eCO_2 studied.

2.1 Introduction

Transpiration contributes a large proportion to global water flows and is therefore an important component of the terrestrial water cycle (Schlesinger and Jasechko, 2014). In particular, a close relationship exists between atmospheric carbon dioxide (CO_2) and transpired water losses (Field et al., 1995). CO_2 concentrations are projected to increase from preindustrial 280 ppm to up to 700-900 ppm by the end of this century (Pachauri et al., 2014). However, there is no clear consensus of the net impact of elevated CO_2 (eCO_2) on the associated transpiration at ecosystem level (Cao et al., 2010; Cheng et al., 2014; Gedney et al., 2006, Manea and Leishman, 2014; Tor-ngern et al., 2015).

To investigate the effect of eCO_2 on transpiration and various feedback mechanisms, free-air carbon dioxide enrichment (FACE) experiments are conducted. They are designed to investigate the impact of eCO_2 on above ground biomass, soil moisture and LAI under field-conditions. In FACE experiments, CO_2 concentrations are increased across a specific area where plants grow under otherwise ambient environmental conditions (Hendrey and Kimball, 1994; Lewin et al., 1994).

A number of studies in which FACE data were used, showed reductions in transpiration under eCO_2 (Cao et al., 2010; Cheng et al., 2014b; Gedney et al., 2006), e.g. by 10.5% at a forest site in Tennessee, USA (*ORNL FACE*, eCO_2: 525~555 ppm) and by 13.8% at a grassland site in Minnesota, USA (*BioCON FACE*, eCO_2: 560 ppm). The reason is a reduced stomatal conductance (g_s) caused by eCO_2 (Field et al., 1995). For example, a significant decline in g_s has been reported for C_3 grasslands by more than 30% on average (eCO_2: ~567 ppm) and for wheat by 35% (eCO_2: 550 ppm) (Ainsworth and Rogers, 2007; Houshmandfar et al., 2015). However, increased CO_2 concentrations are also known to have a fertilizing effect on plants, i.e. plant biomass accumulation is accelerated. Ainsworth and Long (2004) reported an eCO_2-induced increase in above-ground production of 28% for forests and 10% for grasslands (eCO_2: 475-600 ppm). This increase is associated with a higher leaf area index (LAI) and in turn with a higher transpiration. Such an effect of increased LAI is reported to counteract and even offset the water saving effect at leaf level by stomatal closure (Manea and Leishman, 2014; Tor-ngern et al., 2015). However, a higher LAI is further reported to decrease evaporation of grasslands, which results in a net decrease in evapotranspiration (ET) (Liu et al., 2009).

A relationship that summarizes changes in biomass and water consumption is the water use efficiency (WUE), here defined as total above-ground dry biomass (TAB) per water loss through ET. The number of available studies that quantify changes in WUE using FACE data of grassland experiments is limited. However, an increase in WUE is expected and reported by 10 to 32% under eCO_2 (520-550 ppm), depending on crop type and water availability (Deryng et al., 2016; O'Leary et al., 2015; Roy et al., 2016).

Grasslands cover one third of the global terrestrial area (Suttie et al., 2005) and represent an important ecosystem that has been investigated in several grassland FACE experiments (Hovenden et al., 2006; Reich and Hobbie, 2012; Schneider et al., 2004). In a long-term FACE experiment in Giessen, Germany, extensively used grassland has been grown under eCO_2 since 1998, i.e. the eCO_2 concentration was on average 20% higher relative to the aCO_2 (Jäger et al., 2003). The eCO_2 has been reported to increase significantly the TAB in the Giessen FACE rings (Andresen et al., 2017; Kammann et al., 2005). Highest CO_2 effects on TAB have been detected under local average conditions (Obermeier et al., 2017). While an effect of eCO_2 on WUE has been described for the year 2012 (Haworth et al., 2015), the effect of eCO_2 on evapotranspiration and WUE of the temperate, permanent, mown grassland has rarely been investigated and quantified for the long-term.

As often with complex environmental experiments such as FACE experiments, they provide a number of further monitored soil, plant or atmospheric variables making them also ideal for model development, testing and projections. Several modelling studies have addressed the impact of eCO_2 on transpiration (Betts et al., 2007; Gedney et al., 2006; Zaehle et al., 2014) and plant growth (De Kauwe et al., 2013). Recent multi-model intercomparison studies revealed the need for an improved representation of biomass and water balance processes in models for grassland systems (Sándor et al., 2016a, 2016b). Many intrinsic interactions of a variety of ecological, atmospheric and hydrological processes make it difficult to break down the responsible ecophysiological effects leading, for example, to changes in the WUE. Instead of implementing more and more processes into a fixed 'one-model-suits-it-all' code, recent model developments promote flexible programming environments to create tailor-made models for specific sites that allow rigorous hypothesis testing (Clark et al., 2011).

In this study, we use such a coupled hydrological-plant growth model framework to investigate the impact of eCO_2 on a temperate grassland. The coupled model was set up using the Catchment Modelling Framework (CMF) and the Plant growth Modelling Framework (PMF) which represent flexible and integrative tools to build individual models adapted to a specific research question and study site (Houska et al., 2014; Kraft et al., 2011; Multsch et al., 2011). The coupled model has been used in former studies, e.g. to simulate wheat development under different management strategies (Houska et al., 2014). In this study, we further develop PMF by implementing CO_2 response functions and the well-established evapotranspiration module based on Shuttleworth and Wallace (1985) and test the coupled model with the long-term data set of the Giessen grassland FACE site. The use of the coupled model required a number of parameters to be calibrated, leading to parameter uncertainty. In line with Pappenberger and Beven (2006), we think that uncertainty analysis is a prerequisite for any modelling exercise. We therefore applied the established General Likelihood Uncertainty Estimation (GLUE) (Beven and Binley, 1992) method to obtain an estimate of the uncertainty of parameters for the coupled hydrological-plant growth model.

The objective of this study was to investigate the effect of eCO_2 on a temperate grassland's biomass production and water consumption. The complex soil-plant-system was simulated by use of the coupled hydrological-plant growth model. We included the analysis of several hydrological and plant variables, such as TAB, soil water content and WUE with a special focus on transpiration. For robust parametrization, we conducted a sensitivity test followed by an uncertainty analysis under ambient and elevated CO_2 conditions.

2.2 Material and Methods

2.2.1 Study site

This study used long term data (1999 to 2011) from the FACE experiment in Linden (50°32.0'N and 8°41.3'E, 172 m a.s.l.) close to Giessen, Germany. The ongoing experiment was established in 1998 comprising six rings (three control rings with ambient CO_2 (aCO_2): A1, A2, A3 and three with 20% elevated CO_2 (eCO_2): E1, E2, E3) on a grassland research area (Jäger et al., 2003). The rings are paired along a small soil moisture gradient, with dry = A1 and E1, wet = A2 and E2 and intermediate = A3 and E3 (Supporting Information Table S 2-1). However, the vegetation type tall oat-grass (*Arrhenatherum elatioris* – Filipendula ulmaria sub-community) was the same in all rings (Kammann et al., 2005) and was dominated by C3 grasses with 73% of total biomass, followed by forbs with 24% and a small portion of legumes with 3%. The soil is a *Fluvic Gleysol* with a clay layer in altering depths. The soil type is sandy clay loam. Soil porosity varied between 60 and 65% (Kammann et al., 2005). The grassland was not ploughed, but fertilized once a year with 40 kg N ha^{-1} $year^{-1}$.

Model forcing data included meteorological observations (daily sum of precipitation, minimum and maximum temperature, mean wind speed, solar radiation and relative humidity) and groundwater levels. From 1999 to 2011 the area received 573 mm mean annual precipitation and had a mean annual temperature of 9.8°C. The mean CO_2 concentration in the control rings was 394 ppm and in the elevated rings 483 ppm.

Above ground biomass was harvested twice per year (Supporting Information Table S 2-2) and the dry weight was taken for model evaluation. During the observation period, the mean dry matter in harvested biomass for ambient rings was about 399.5 (± 100.3) at the first and 263.6 (± 47.2) g m^{-2} at the second harvest. The mean dry matter in harvested biomass for elevated rings was 425.5 (± 93.6) and 294.2 (± 54.3) g m^{-2}. We used soil moisture data for model testing, which was measured at a depth of 0.15 m below the soil surface during several days a week. Volumetric soil water content was about 37.0% (± 11.3) and 38.4% (± 10.4) on average for ambient and elevated rings, respectively. Since the hydrological model did not account for changes of the aggregate state of soil water during frost periods, frost days during the winter period were not considered for model evaluation.

2.2.2 Model setup

For detailed simulation of the soil hydrological and plant growth processes two independent generic, deterministic models were set up and coupled. The hydrological model and the plant growth model were set up using the Catchment Modelling Framework, CMF (Kraft et al., 2011), and the Plant growth Modelling Framework, PMF (Multsch et al., 2011), respectively. Both modelling frameworks represent flexible and integrative tools to build individual models adapted to a specific research question and study site. For instance, the coupled model has been used to simulate wheat development under different management strategies (Houska et al., 2014).

2.2.2.1 Catchment Modelling Framework: CMF

CMF is a flexible modelling framework which can be used to set up individual hydrological models, e.g. a 1-dimensional soil column, a fully integrated 3-dimensional landscape model or a lumped catchment model. The core classes and functions of CMF are implemented in C++ and can be linked by using the Python programming language, which serves as an interface for using CMF. For the simulation of the FACE experiment in this study a 1-dimensional model was set up. The soil column was set to a depth of 1.7 m to capture ground water levels and was subdivided into 18 layers. The soil column started with 0.01 m thickness for the first layer for an adequate representation of small scale processes in the upper soil layers and continued with rising thickness by 0.01 m with depth, i.e. 0.02 m thickness for second layer, 0.03 m for third layer, etc. Water flux was simulated by applying the Richards' equation (Richards, 1931). Soil hydraulic properties were described with the van Genuchten-Mualem function (van Genuchten, 1980) and characterized by saturated conductivity (k_{sat}), porosity (φ), the pore size distribution parameter (n) and the inverse of water entry potential (α). For simplicity, the 18 layers were described with the same parameter values. Measured groundwater levels and precipitation were used as forcing data.

2.2.2.2 Plant growth Modelling Framework: PMF

PMF divides the plant into the components root, shoot, stem, leaves and reproductive organs. Different biophysical process representations are available in a Process Library to simulate plant growth (Multsch et al., 2011). Plant development is calculated on the basis of the thermal time concept (Monteith and Moss, 1977) and affected by day length (Zheng et al., 2014). Biomass accumulation is simulated according to the radiation use efficiency-concept (Monteith and Moss, 1977), which transforms absorbed photosynthetically active radiation into dry matter. Accumulated biomass is distributed to the plant components depending on the actual growth stage. Root growth is simulated by daily partitioning of root biomass between soil layers and limited by the soil moisture in each layer. Water uptake is calculated for each soil layer according to the root biomass distribution. Taking into account wet and dry conditions, a stress function according to Feddes et al. (1978) returns a water stress factor for each layer.

2.2.2.3 Coupling of CMF and PMF

The Python programming language was used to couple the models as recommended for scientific research by Perkel (2015). Overall, PMF simulated ET and biomass accumulation including LAI development on time step *t* considering states of CMF at *t*-1, called operator split. Subsequently, CMF continued taking into account calculated plant water demand and considered partitioning of precipitation due to changes in interception capacity in the course of leaf development. The detailed processes in each model are described in the next sections.

2.2.2.4 Further development of PMF

For the simulation of the potential effect of eCO_2 on biomass and transpiration, PMF has been enhanced by implementing a well-established ET module (Shuttleworth and Wallace, 1985) and a CO_2 response function (Soltani and Sinclair, 2012).

The Shuttleworth and Wallace (1985) (SW) equation determines evaporation and transpiration on a network of coupled resistances. The set of SW-equations was implemented according to Zhou et al. (2006) (Supporting Information Text S 2-1). The stomatal resistance r_s^c [s m^{-1}] combines the counteracting impact of increased LAI and stomata closure. As implemented in PMF, the resistance was governed by combinations of simple linear response functions to air temperature ($temp_{res}$), vapor pressure deficit (vpd_{res}) and atmospheric CO_2 concentrations (co_{2res}) (eq. 2-1). Each response function returns a value between 0 and 1. The function was 0 when stomata were closed and 1 when stomata were maximally opened. An increase in air temperature lead to higher values for $temp_{res}$, whereas an increase in atmospheric CO_2 or vapor pressure results in lower values for vpd_{res} and co_{2res}, respectively:

$$r_s^c = r_{min}^{st} / \left(lai_{eff} \left(temp_{res}\ vpd_{res}\ co_{2res} \right) \right) \tag{2-1}$$

where lai_{eff} is the effective leaf area index [$m^2\ m^{-2}$] which constraints the portion of LAI that is active in transfer of vapor and heat. According to Gardiol et al. (2003) the lai_{eff} is defined to be equal to LAI as long as LAI ≤ 2. If LAI is between 2 and 4, the lai_{eff} is equal 2 and if LAI ≥ 4 the lai_{eff} is equal to 0.5*LAI. r_{min}^{st} is defined as the minimum stomatal resistance of individual leaves under optimal conditions [s m^{-1}]. The linear response functions to temperature (eq. 2-2) and vapor pressure (eq. 2-3) were taken from Zhou et al. (2006) and the response to CO_2 (eq. 2-4) was implemented according to Stöckle (1992) and Wu et al. (2012):

$$temp_{res} = 1.0 - \left(1.6 \times 10^{-3} \left(298 - \left(temp_{meas} - 273.16 \right) \right) \right) \tag{2-2}$$

$$vpd_{res} = 1.0 - 0.409\ (e_s - e_a) \tag{2-3}$$

$$co_{2res} = (1 + p) - p\ co_{2meas} / co_{2ref} \tag{2-4}$$

where $temp_{meas}$ is the measured air temperature [°C], e_s the saturated vapor pressure [kPa], e_a the actual vapor pressure [kPa], p is a constant regulating the stomatal response to eCO_2 when $co_{2meas} \neq co_{2ref}$, co_{2meas}

the measured atmospheric CO_2 concentration [ppm] and co_{2ref} the reference CO_2 concentration, here 394 ppm.

To simulate the impact of eCO_2 on plant biomass accumulation, a response function was implemented (Soltani and Sinclair, 2012) which increases the radiation use efficiency (RUE), i.e. the amount of biomass growth in relation to photosynthetic active radiation, depending on the measured CO_2 concentration co_{2meas}:

$$rue_{CO2} = rue_{ref}\left(1.0 + b \ln\left(co_{2meas}/co_{2ref}\right)\right) \quad (2\text{-}5)$$

where rue_{CO2} is in [g MJ^{-1}], rue_{ref} is the radiation use efficiency at reference level of 394 ppm in [g MJ^{-1}] and b is a constant regulating the response of RUE to eCO_2 when $co_{2meas} \neq co_{2ref}$.

2.2.3 Sensitivity analysis

We conducted the Fourier amplitude sensitivity test (FAST) based on Saltelli et al. (1999) to identify the most sensitive parameters. The FAST method allows the calculation of each input factor's contribution to variance of the output. Here, the considered eighteen input factors were fourteen plant specific parameters influencing biomass accumulation, plant development and evapotranspiration and four van Genuchten-Mualem parameters. A minimum number of 39,000 model runs was estimated for the FAST algorithm (Henkel et al., 2012). With these model runs, 11 parameters were identified as most sensitive parameters (Supporting Information Table S 2-3) and only those 11 parameters were further considered for the GLUE analysis. The sensitivity test was conducted using the recently developed open source python package SPOTPY (Houska et al., 2015). Further details concerning the conducted FAST procedure are depicted in the Supporting Information Figure S 2-1.

2.2.4 Parametrization and uncertainty analysis

GLUE was first defined by Beven and Binley (1992) and follows the concept of equifinality, i.e. the basic idea is that different parameter sets can lead to 'behavioural', equally acceptable model runs. The parameter sampling is commonly carried out by Monte Carlo sampling. To improve sampling, the Latin Hypercube (LH) algorithm by (McKay et al., 1979) was used. The GLUE analysis was conducted to calibrate the model for the years 1999-2011 using SPOTPY (Houska et al., 2015).

In the first step, the prior distribution was created. A uniform distribution was assumed for the 11 parameters, with the benefit of needing no prior knowledge about proved parameter optima and with the cost of possible loss of efficiency to generate behavioural model runs. Using LH sampling 100,000

parameter sets, i.e. the prior distribution, were generated and used to simulate the ambient FACE rings. The 100,000 model runs represented a trade-off between runtime and parameter space.

In the second step, the posterior distribution was created. For this, simulated above ground biomass and soil moisture were compared with observed data by using six objective functions (three for each output variable). Only parameter sets fulfilling all user-defined criteria as listed in Table 2-1 were regarded as behavioural runs, which built up the posterior distribution.

Table 2-1: User-defined criteria used for GLUE analysis. Only simulations fulfilling these were considered for further analysis.

	r^2	**bias**	**RMSE**
soil moisture	>0.3	<10 vol.%	<10 vol.%
biomass	>0.3	<80 g dry matter m^{-2}	<150 g dry matter m^{-2}

The GLUE method was conducted twice for ambient and twice for elevated rings. On basis of the results of the first GLUE, the parameter ranges were adapted, which increased the number of posterior parameter sets of the second GLUE for all rings (Table 2-2). The multiple GLUE analysis for ambient and elevated parameter resulted in 82 remaining model runs for the ambient rings A1-A3 and in 1398 for the elevated rings E1 and E3 (i.e. 82 sets extended by several combinations of the CO_2 response factors *p* and *b*). Ring E2, which was the wettest ring, was rejected during the GLUE analysis and was therefore excluded in further analyses.

Detailed descriptions of the objective functions and the conducted multiple GLUE analyses are available in the Supporting Information Text S 2-2 and Text S 2-3.

In addition to the GLUE analysis, the effects of different levels of *b* and *p* on TAB and transpiration, respectively, were tested. For this, *b* and *p* were varied from 0.0-0.5 and the other parameters were set to fix values as listed in the Supporting Information Table S 2-5.

Table 2-2: Parameters as used for the multiple GLUE analysis including parameter name, description, unit and range. Based on the results of the 1. GLUE, narrowed parameter ranges were used for the 2. GLUE.

Parameter	**Description and unit**	**1. GLUE**		**2. GLUE**	
		Min	**Max**	**Min**	**Max**
α	inverse of the air entry potential [cm^{-1}]	0.001	0.7	0.2	0.6
b*	constant regulating response of RUE to [CO_2]	0	2	0.0	0.6
c_r	leaf extinction coefficient [-]	0	0.8	0	0.5
k_{sat}	saturated conductivity [m day^{-1}]	0.1	25	13	25
$leafweight_s$	specific leaf weight [g m^{-2}]	20	90	20	90
n	shape parameter of retention curve, empirical [-]	1.1	1.5	1.1	1.2
p*	constant regulating stomatal response to [CO_2]	0	0.5	0.0	0.5
rootgrowth	root elongation factor [cm d^{-1}]	0.15	2.9	0.15	2.9
rue_{ref}	radiation use efficiency at 394 ppm CO_2 [g MJ^{-1}]	2.4	3	2.4	3
r^{st}_{min}	min stomatal resistance of individual leaves under optimum conditions [s m^{-1}]	50	150	40	80
t_{base}	min temperature for plant growth [°C]	1	9	1	5
$tt_{emergence}$	thermal time at emergence [°days]	70	150	70	120
$tt_{tillering}$	thermal time at end of tillering [°days]	200	463	200	340

* only relevant under eCO_2

2.3 Results

2.3.1 Model performance

The coupled model showed a good performance in predicting biomass with an r^2 between 0.3 and 0.6 in combination with a bias ranging between 0 and 80 g dry matter m^{-2} for the five different FACE rings, indicating a slight overestimation of biomass (Supporting Information Table S 2-4). An outlier was the year 2005, where at first harvest TAB was overestimated by 1.8 times compared to field observations (Figure 2-1a-e).

Generally, a pattern of higher yields at first harvest and lower yields at second harvest was simulated, which is consistent with measured data. Moreover, the simulations resulted in a significant increase in TAB of about 6.5% ($p < 0.001$, two-sided t-test for related samples) under eCO_2, which is in line with the significant increase in observed biomass (+9.1%). However, a simulated increase in TAB by 9% and 2% at first and second harvest in comparison to an observed increase by 6% and 13%, respectively, showed limitations in a harvest-wise analysis of the CO_2 effect.

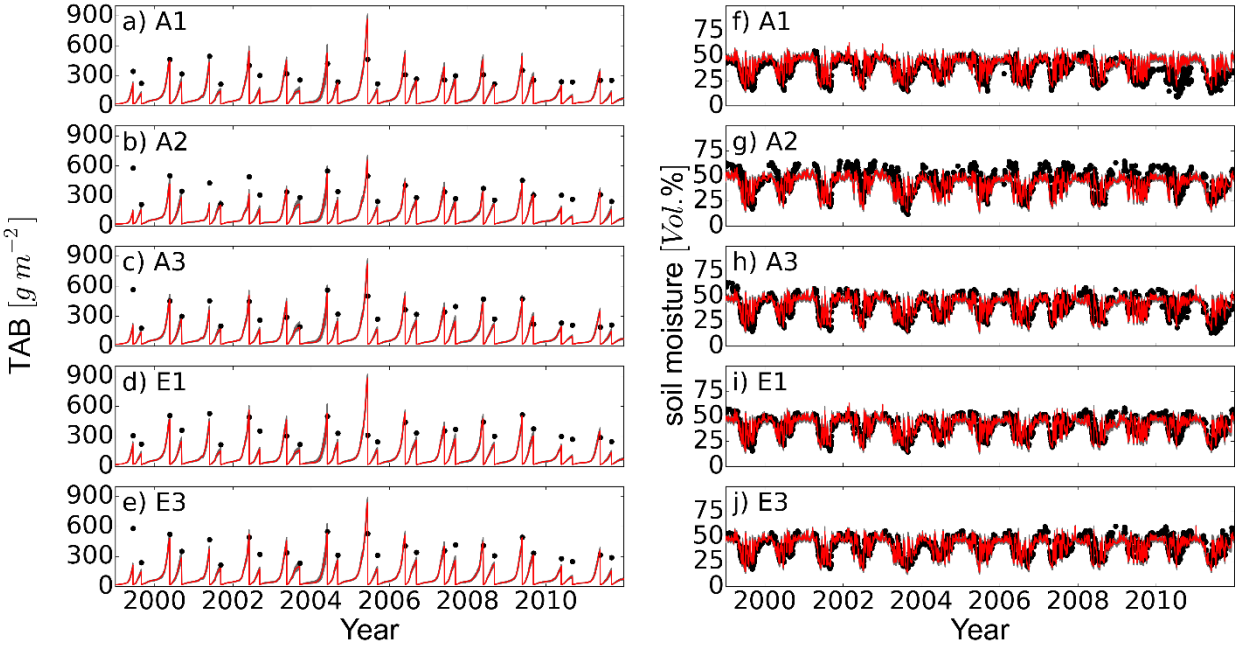

Figure 2-1: Time series of TAB and soil moisture. Observed as well as simulated TAB (a-e) and soil moisture (f-j) in each ring (aCO_2: A1, A2, A3 and eCO_2: E1, E3) using the posterior distribution. Observed data: black dots; simulated data: median (red line) and uncertainty (grey area, where lower and upper boundary are 5% and 95% percentile).

The pattern of higher soil moisture during winter and lower soil moisture in summer months was well represented in each ring (Figure 2-1 f-j). The model showed a good performance, reflected by the values of the respective objective functions: r^2 between 0.4 and 0.7 in combination with low bias of -7 vol.% to 0 vol.% and an RMSE ranging between 6 vol.% and 10 vol.% (Supporting Information Table S 2-4). However, in periods of saturated soil conditions, i.e. where measured soil water content was >60 vol.%, the model tended to underestimate the observations by about 14 vol.% on average. eCO_2 led to no decrease of the long-term soil moisture content (-0.3 vol.%). This is in line with the observed data (+0.3 vol.%).

2.3.2 Parameter distribution and uncertainty

The GLUE analysis revealed improved parameter ranges and parameter distributions (Table 2-2 and in the Supporting Information Figure S 2-2). The range of *b* (eq. 2-5), for instance, was narrowed by 75% from prior 0-2, showing values mainly between 0.1 and 0.3 after the second GLUE. The parameter *p* (eq. 2-4), which determined the sensitivity of stomatal conductance to eCO_2, revealed a maximum at 0.3. Further optima became visible, e.g. for the parameters *n*, t_{base}, c_r and rue_{ref} at 1.12 [-], 3.5°C, 0.27 [-] and 2.5 [g MJ^{-1}]. Specific distributions can be used to sample values for the prior distribution instead of a uniform distribution for further analysis. For example, the parameter distribution of rue_{ref} was skewed to the right. The GLUE method requires that the parameters do not correlate (Jin et al., 2010) which has been proven by visual inspection of scatter plots (Supporting Information Figure S 2-3).

The uncertainty range of TAB was on average 19 g dry matter m^{-2}, being low during winter periods and increasing towards the harvest dates. The uncertainty range of the predicted soil moisture was constant at 5% using the 5 to 95% percentiles of the posterior simulations.

A one-at-a-time uncertainty analysis was conducted to investigate the effect of different levels of the parameter *b* and *p* on the simulated TAB and transpiration, respectively. An increase of parameter *b* from 0.0-0.5 resulted in an increase in TAB and led to an uncertainty range in TAB at harvest of 98.6 ± 30.8 g dry matter m^{-2} (Figure 2-2a). A stepwise increase of parameter *p* from 0.0-0.5 decreased transpiration and resulted in an uncertainty range of 12.5 ± 2.1 mm (Figure 2-2b).

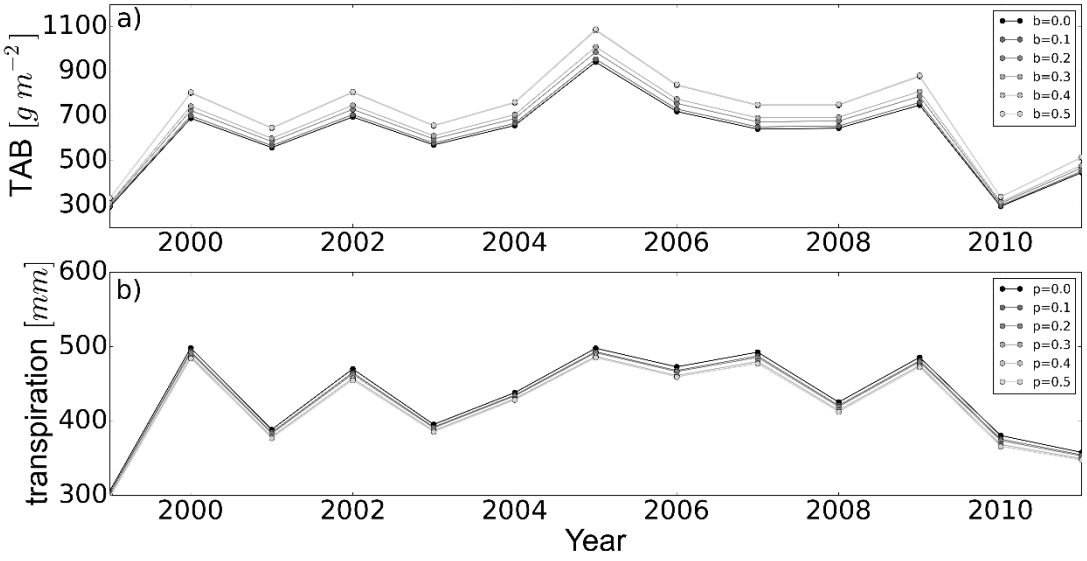

Figure 2-2: Effect of different levels of parameter *b* on the simulated TAB (a) and different levels of parameter *p* on the simulated transpiration (b) of the FACE ring E1.

2.3.3 CO_2 effect on water use efficiency

WUE was calculated for the entire growing season and derived by dividing annually harvested TAB by accumulated ET (from March to second harvest in September). A two-sided t-test for related samples was used to test for significant differences. The simulated TAB was on average about +40.7 ±24.0 g dry matter m^{-2} (6.5%) higher under eCO_2 compared to aCO_2. ET remained with 0.9 ±4.9 mm (+0.2%, p = 0.5), evaporation was significantly reduced by -2.1 ±1.7 mm (-1.4%, p < 0.01), whereas according to our simulations transpiration increased on average by +3.0 ±6.0 mm (+0.8%, p = 0.1) during the growing season (Figure 2-3).

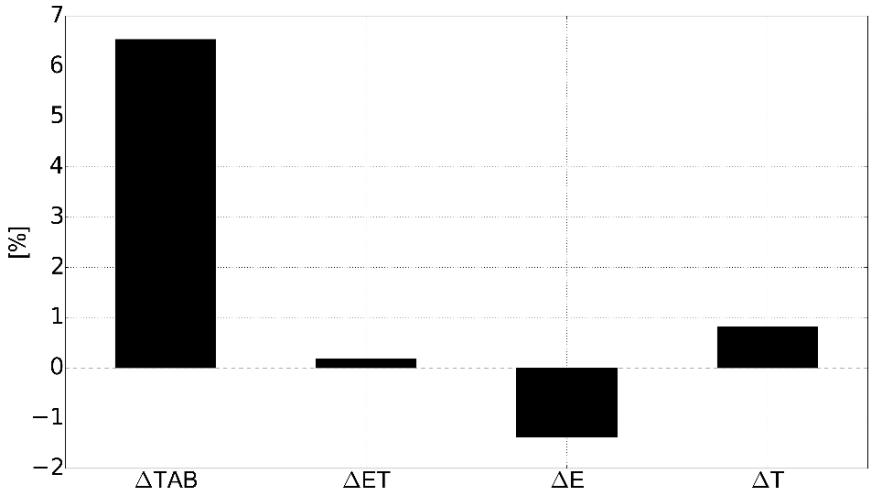

Figure 2-3: Simulated mean differences between ambient and elevated TAB (ΔTAB), ET (ΔET), evaporation (ΔE) and transpiration (ΔT) in [%] at the grassland FACE site in Giessen, Germany, for the years 1999-2011.

On average, the WUE was at ~2.5 kg m^{-3}. An inter-annual variability of WUE was revealed by a minimum of 1.3 (in year 2010) and a maximum of 3.2 kg m^{-3} (in year 2005). The uncertainty range for WUE was equal for both CO_2 treatments (0.7 kg m^{-3}), i.e. not increasing under eCO_2 using the 5 to 95% percentiles of the posterior simulations (Figure 2-4).

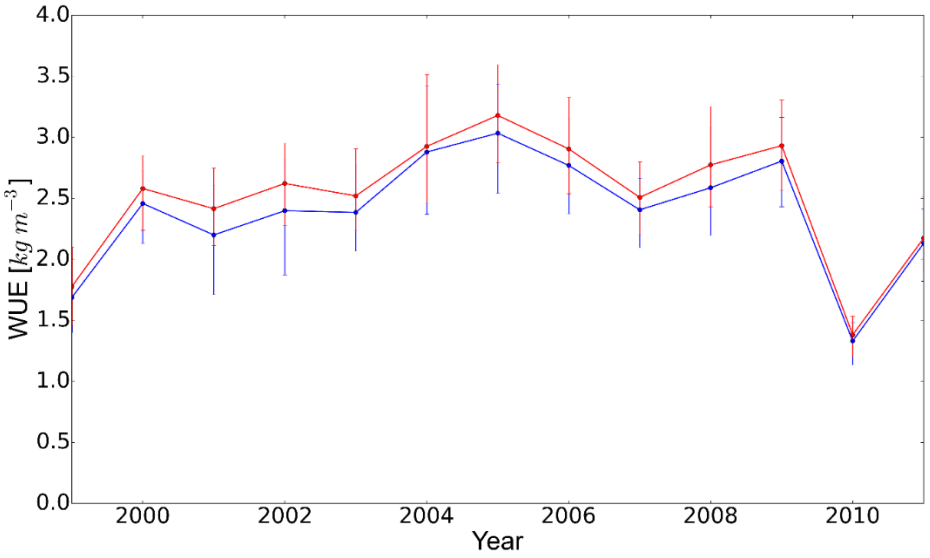

Figure 2-4: Absolute WUE over time. Simulated WUE [kg m^{-3}] at the grassland FACE site in Giessen, Germany. Median through simulations (aCO_2 = blue line, eCO_2 = red line), uncertainty with 5% and 95% percentile as lower and upper limit (aCO_2 = blue error bar, eCO_2 = red error bar).

On average a significant increase in WUE of 5.2% (0.1 ±0.06 kg m^{-3}, $p < 0.001$) was found under eCO_2. The positive impact of eCO_2 on WUE was apparent for all years (Figure 2-5). Thus, the improvements in TAB (+6.5%) in combination with the remained ET (+0.2%) led to an overall better performance of the WUE. In particular, the strongest effect occurred in 2001 (10.0%) and 2002 (9.5%) despite of increased water loss through ET (+0.6 and +2.0%). The smallest effect on WUE appeared in 2004 (2.0%) in line with smallest effect on TAB.

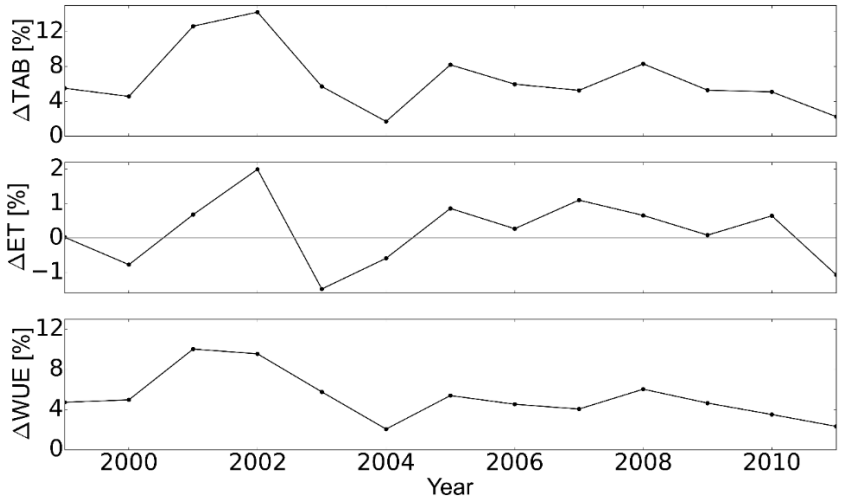

Figure 2-5: Relative change in TAB, ET and WUE over time. Impact of eCO_2 on TAB, ET and WUE [%] at the grassland FACE experiment in Giessen, 1999-2011, Germany.

2.4 Discussion

2.4.1 Model performance

The Giessen FACE experiment is unique in investigating the effect of eCO_2 over more than 18 years (since 1998, still ongoing) using a moderate carbon dioxide fumigation level of 20% increase for a temperate well-watered grassland. Taking the low CO_2 enrichment at the Giessen study site in comparison to other FACE sites (Haworth et al., 2015), the predicted increase in TAB of about 6.5% under 20%-elevated CO_2 is slightly lower compared with the meta-study by Ainsworth and Long (2004). They investigated different grassland FACE studies (eCO_2: 475 - 600 ppm) resulting in an average increase of TAB of about 10%.

Fitting the hydrological-plant growth model to the observed data by conducting the GLUE method showed that the coupled CMF-PMF model matched the observed TAB (r^2 between 0.3 and 0.6, bias between -80 and 0 g dry matter m^{-2}, RMSE between 122 and 150 g dry matter m^{-2}). The obtained r^2 between 0.3 and 0.6 showed a better performance in comparison with results of a multi-model comparison by Sándor et al. (2016b) who reported a $r^2<0.3$ for grassland biomass simulation. The RMSE is in line with O'Leary et al. (2015), who investigated the model performance of six wheat models under aCO_2 and eCO_2. The study resulted in an r^2 between 0.56 and 0.64 for biomass and in a RMSE from 140 to 150 g m^{-2}. However, other studies resulted in ranges with a lower RMSE, e.g. Moot et al. (2015) who calibrated the APSIM model for 'Grasslands Kaituna' lucerne with a resulting RMSE of 65 g m^{-2}. Pequeno et al. (2014) simulated biomass accumulation of Marandu palisade grass in Brazil under irrigated and rain fed conditions showing a RMSE between 46 and 53 g dry matter per m^2. At the first harvest in 2005, the model predicted a peak in TAB in each of the FACE rings (Figure 2-1). This is contrary to the observed data because the predicted TAB is 1.6 fold higher. A likely reason for this is that biomass accumulation had reached its capacity limit, which was not captured by the plant model.

In recent studies, the presentation of accurate soil water processes had been identified as a challenge in modelling grassland ecosystems with r^2 reported between 01. and 0.7 (Sándor et al., 2016a, 2016b). The coupled CMF-PMF showed a good performance in predicting soil moisture (r^2 between 0.4 and 0.7, bias of -7 vol.% to 0 vol.% and an RMSE ranging between 6 vol.% and 10 vol.%). Nendel et al. (2009), who used the HERMES model in combination with a six year long data set of FACE experiment on different crops in Braunschweig, Germany, tested different CO_2 response algorithms and reported a mean average error in soil moisture between 9.9 and 14.4% and a bias ranging from minimum 2.4 to maximum -7.4%. Houska et al. (2015) presented a bias of 2% in the upper 0.3 m and a higher r^2 of 0.8 for the A1 ring of the FACE experiment in Giessen. As stated above, in periods where data showed almost saturated conditions (between 60-65 vol.%) the coupled model did not match observed soil moisture. We want to point out that different

sources might have contributed to this divergence, a) the general limitation in soil moisture simulation under almost saturated conditions using the van Genuchten-Mualem analytical function (Schaap and Van Genuchten, 2006), b) the simplified representation of soil parameters for the entire soil and c) potentially larger errors in observed data at high soil water content (IMKO Micromodultechnik GmbH, 2001).

The PMF model provides a detailed root growth mechanism, i.e. the biomass is allocated between the different soil layers according to the soil water and nutrient supply. The simulations indicated increased root biomass when comparing aCO_2 and eCO_2. This is in line with the observation from Carrillo et al. (2014) who reported an increase in root biomass of about 30% induced by eCO_2 (600 ppm). Roy et al. (2016) observed a significantly increased root growth by 77% under eCO_2 (520 ppm). In addition to increased root biomass production, the predominant allocation of the biomass in upper soil layers, as described for soybeans under eCO_2 by Gray et al. (2016), could play an important role in affecting the water budget. However, there was no plant biomass data of single plant components, in particular roots, available for validation.

2.4.2 Parameter distribution and uncertainty

The GLUE analysis revealed the uncertainty range of soil moisture with 5% and of TAB with 19 g dry matter m^{-2}, which was related to parameter selection. The parameter *b* that determines the RUE response to eCO_2 was between 0.1 and 0.3 at the C3 grassland FACE site in Giessen (Supporting Information Figure S 2-2). Parameter *p* that determined the stomatal response to eCO_2 was set to a fixed value of 0.4 in a study by Stöckle (1992) and was later adapted to 0.24 for pastures with C3 grasses (Wu et al., 2012). In this study, *p* reached its maximum at 0.3 for the C3 grassland in Giessen, Germany. The extinction coefficient of vegetation c_r appeared to have its mathematical maximum at values <0.3. This is in contrast to other studies, where c_r has been set to fixed values between 0.5 and 0.9 (Lantinga et al., 1999; Sándor et al., 2016b; Shuttleworth and Wallace, 1985). A decrease in c_r results in reduced biomass production. Hence, we suppose that by sampling small c_r-values the model covered a stress factor which was not explicitly included in the model but which occurred in the field, e.g. nitrogen stress or competition for light and space.

Other sources of uncertainty, i.e. of input data and model structure, have not been investigated in this study. For example, Nendel et al. (2009) tested six different CO_2 response algorithms, i.e. model structure, and showed only small differences in the performance. They reported an index of agreement ranging between 0.94 and 0.99 for above ground dry matter and between 0.82 and 0.86 for soil moisture. Nevertheless, the need for improved model structures, i.e. improved representation of biomass production, soil temperature and soil water content, to reduce uncertainty is shown by a multi- model intercomparison project for

grassland models (Houska et al., 2017; Ma et al., 2014; Sándor et al., 2016a, 2016b) and by the vast number of model intercomparison studies on wheat (Asseng et al., 2014; Kollas et al., 2015; Rosenzweig et al., 2014, 2013; Rötter et al., 2012). Moreover, the utilization of benchmark datasets for growth models as presented by Asseng et al. (2015) is helpful to identify uncertainties.

2.4.3 CO_2 effect on water use efficiency

A distinct increase in TAB was predicted in this study for the temperate grassland study site, while the ET was predicted to remain the same. These predictions are in line with other studies (Ainsworth and Long, 2004; Leakey et al., 2009). Splitting the ET into evaporation and transpiration revealed a decrease in evaporation and a net increase in transpiration. This is in line with a study by Liu et al. (2009) who studied effects of expanded grassland on vegetation-soil moisture feedback. They report an increase in transpiration, whereas evaporation was reduced as a consequence of reduced soil evaporation. The increase in transpiration means that the decrease in stomatal conductance as a consequence of eCO_2 at the leaf level was counteracted at the stand level by the rise of the effective leaf area index (lai_{eff}). Manea and Leishman (2014) reported comparable results and described an offset of the stomatal effect in a temperate grassland due to an increase in leaf area index under eCO_2.

The coupled CMF-PMF predicted an increase in WUE of 5.2% on average under eCO_2 for the grassland research area in Giessen. This is lower in comparison to the global increase in crop water use of 10-27% under 550 ppm as presented by Deryng et al. (2016). Further, O'Leary (2015) predicted an increase in WUE for wheat under eCO_2 (ambient 365 ppm vs elevated 550 ppm) of more than 30%, defining WUE as produced grain yield per water loss including ET, deep drainage and run-off. De Kauwe et al. (2013) reported an observed increase of 66% and 93% under eCO_2 (542 ppm and 547 ppm) for a conifer and a deciduous forest. A predicted significant increase of 5.2% at the Giessen FACE site is reasonable considering the moderate CO_2 fumigation level of ~480 ppm. However, we conclude that more research with focus on CO_2-induced change in WUE of temperate grasslands is necessary, including studies with moderate levels of eCO_2.

2.4.4 Conclusion

We show that the coupled hydrological-plant growth model is a robust tool for the investigation of CO_2 effects of a permanent, temperate grassland system. In future studies, further grassland sites, crops and treatments, e.g. combined eCO_2 x water regime studies, will be tested. In contrast to a number of prior studies, the current study reports a simulated increase in the transpiration of the temperate grassland under

eCO_2. Thus, the expected water saving effect at the leaf level, caused by stomatal closure, was offset at the stand level, caused by the significantly increased TAB of the grassland. However, the net ET was simulated to remain the same under eCO_2, as transpiration increased but soil evaporation significantly decreased. Finally, the combination of significantly increased TAB and constant net ET resulted in a significant increase in WUE under eCO_2. Our results indicate that mown, temperate, wet-dry grasslands can benefit from enhanced biomass accumulation while maintaining water consumption already at a 20% increase in CO_2 concentrations.

Acknowledgements

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Supporting Information

Table S 2-1: Averaged, observed soil moisture [Vol%] plus standard deviation (std) in the six FACE ring over the years 1999-2011.

	A1	**A2**	**A3**	**E1**	**E2**	**E3**
mean	32.7	42.6	36.0	37.2	40.5	37.5
std	9.4	11.8	10.3	9.7	11.6	9.4

Table S 2-2: Harvest dates from 1999-2011 at the grassland FACE site in Giessen, Germany.

	First harvest	**Second harvest**
1999	June 14	August 31
2000	May 23	September 11
2001	May 28	September 10
2002	June 3	September 09
2003	May 19	September 18
2004	June 1	September 06
2005	June 13	September 13
2006	May 29	September 11
2007	May 30	September 10
2008	May 27	September 8
2009	May 25	September 7
2010	May 25	September 6
2011	May 23	September 5

Table S 2-3: Overview of the 18 parameters that were considered for sensitivity test (FAST) covering the parameter's name, definition and unit as well as the defined lower and upper limit. FAST identified 11 most sensitive parameters (bold). Parameters that were not sensitive were assigned to fixed values (not bold). These values are presented in column 'Fixed'.

Parameter	**Description and unit**	**Ranges**		**Fixed**
		Min	**Max**	
α	**inverse of the air entry potential, empirical [cm^{-1}]**	**0.001**	**0.7**	
Φ	porosity [-]	0.6	0.65	0.63
c_r	**leaf extinction coefficient [-]**	**0.0**	**0.8**	
k_{sat}	**saturated conductivity [m day^{-1}]**	**0.1**	**25**	
$leafweight_s$	**specific leaf weight [g m^{-2}]**	**20**	**90**	
n	**shape parameter of retention curve, empirical [-]**	**1.1**	**1.5**	
rootgrowth	**root elongation factor [cm d^{-1}]**	**0.15**	**2.9**	
rue_{ref}	**radiation use efficiency at 394 ppm CO_2 [g MJ^{-1}]**	**2.4**	**3**	
r^{st}_{min}	**min stomatal resistance of individual leaves under optimum conditions [s m^{-1}]**	**50**	**150**	
$tt_{anthesis}$	thermal time at end of anthesis [°days]	900	1091	996
t_{base}	**min temperature for plant growth [°C]**	**1**	**9**	
$tt_{emergence}$	**thermal time at emergence [°days]**	**70**	**150**	
$tt_{leafdevelopment}$	thermal time at end of leaf development [°days]	150	200	175
$tt_{maturity}$	thermal time at maturity [°days]	1672	1832	1752
$tt_{ripening}$	thermal time at end of ripening [°days]	1291	1672	1480
$tt_{seedfilling}$	thermal time at end of seed filling [°days]	1091	1291	1191
$tt_{stemelongation}$	thermal time at end of stem elongation [°days]	700	900	800
$tt_{tillering}$	**thermal time at end of tillering [°days]**	**200**	**463**	

Table S 2-4: Best and worst results of the objective functions for the two output variables soil moisture and TAB for the rings A1, A2, A3, E1 and E3.

		Soil moisture [%]					**TAB [g m^{-2}]**				
		A1	A2	A3	E1	E3	A1	A2	A3	E1	E3
r^2	best	0.52	0.69	0.68	0.70	0.70	0.60	0.40	0.49	0.42	0.54
	worst	0.43	0.44	0.52	0.56	0.55	0.49	0.30	0.37	0.31	0.44
bias	best	-0.08	0.80	-0.03	0.00	-0.01	0.43	21.05	-0.52	0.02	2.97
	worst	-7.07	6.48	-4.51	3.74	-3.07	-49.11	79.88	35.64	53.30	69.83
RMSE	best	6.88	7.29	5.97	5.63	5.51	109.13	116.40	117.52	132.85	122.43
	worst	9.99	9.98	8.03	6.93	7.04	145.42	133.40	133.83	150.00	136.52

Table S 2-5: Selected parameter set that was used for the uncertainty analysis of the parameters *b* and *p*.

Parameter	**Description and unit**	**Value**
α	inverse of the air entry potential [cm^{-1}]	0.25
c_r	leaf extinction coefficient [-]	0.14
k_{sat}	saturated conductivity [m day^{-1}]	18.41
leafweight$_s$	specific leaf weight [g m^{-2}]	39.05
n	shape parameter of retention curve, empirical [-]	1.12
rootgrowth	root elongation factor [cm d^{-1}]	1.66
rue_{ref}	radiation use efficiency at 394 ppm CO_2 [g MJ^{-1}]	2.52
r^{st}_{min}	min stomatal resistance of individual leaves under optimum conditions [s m^{-1}]	53.66
t_{base}	min temperature for plant growth [°C]	4.76
$tt_{emergence}$	thermal time at emergence [°days]	101.8
$tt_{tillering}$	thermal time at end of tillering [°days]	200.6
b	constant regulating response of RUE to [CO_2]	0.0-0.5
p	constant regulating stomatal response to [CO_2]	0.0-0.5

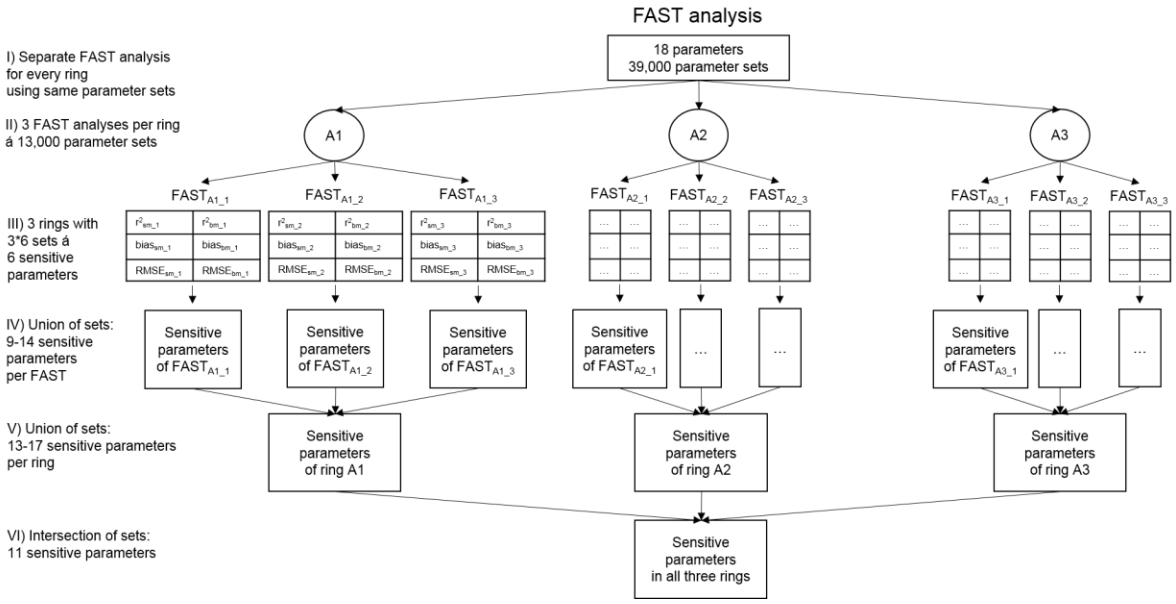

Figure S 2-1: Overview of conducted FAST. Steps conducted to identify the most sensitive parameters occurring in the three FACE rings A1, A2 and A3. The sensitivity test (FAST) covers 4 hyrological and 14 plant model related parameters. 39,000 parameter sets were created on the basis of the FAST algorithm. Every ring was then tested with the 39,000 parameter combinations. Due to computer capacity three FASTs with 13,000 parameter sets per ring were conducted. The union of sets resulted in the most sensitive parameters per ring. Finally, the intersection of sets identified those sensitive parameters that occurred in every ring.

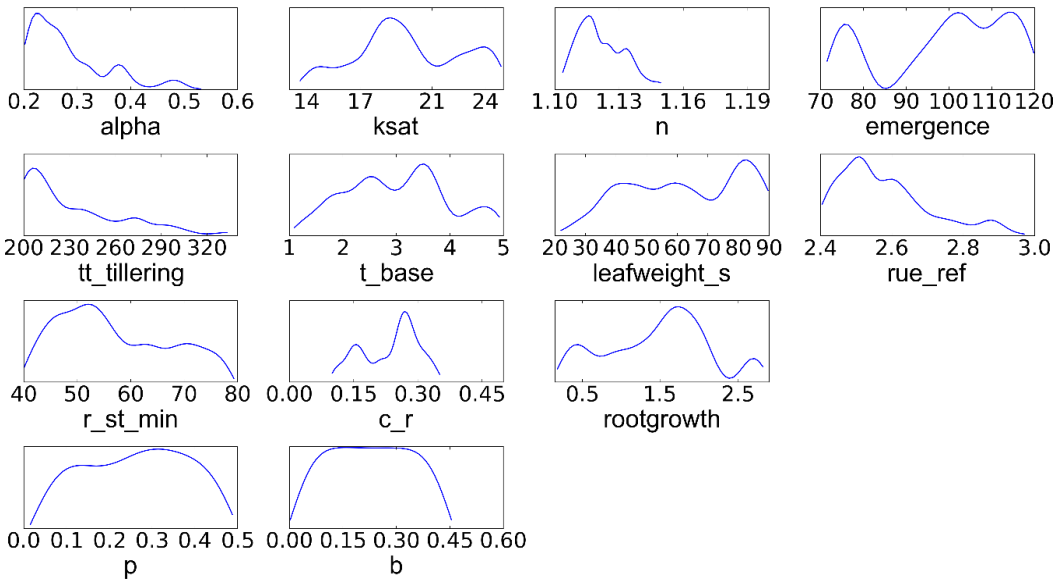

Figure S 2-2: Parameter distribution plot. Parameter distribution of posterior parameter sets of the FACE rings A1-A3, E1, E3. For parameter acronyms see Table S 2-5 in the Supporting Information.

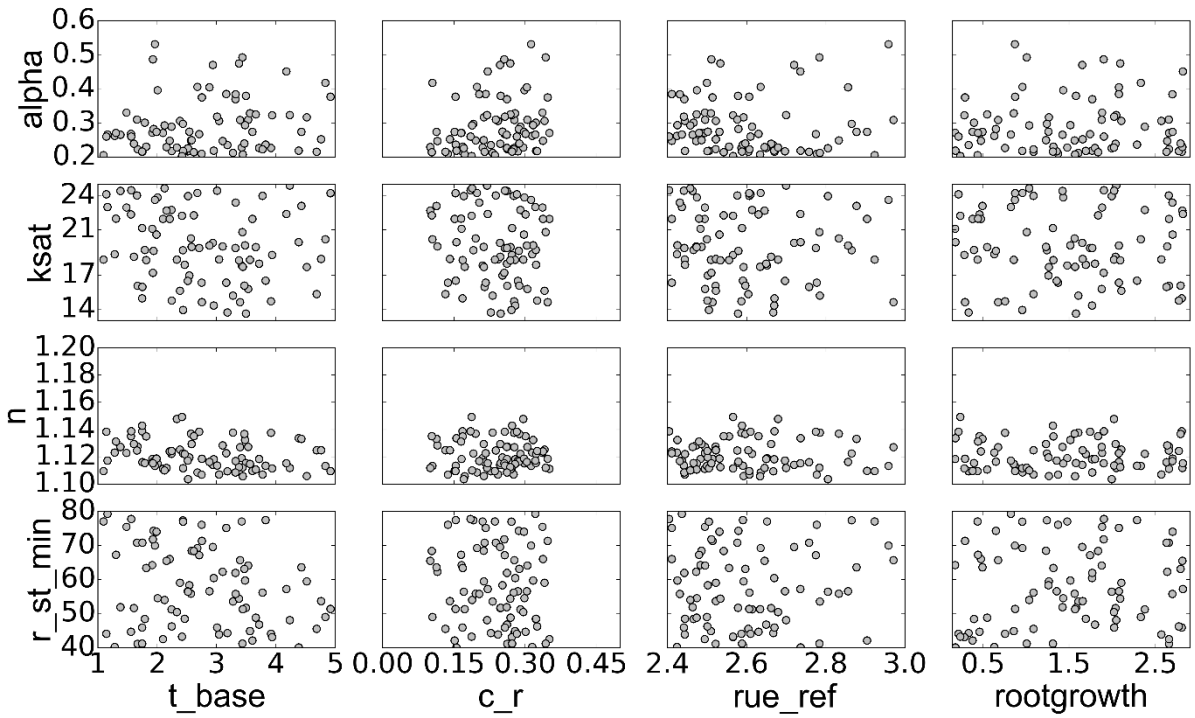

Figure S 2-3: Parameter interaction plot. Parameter interaction and distribution of posterior parameter sets of the FACE rings. The items on the x-axis and y-axis show plant and soil hydraulic parameters. For parameter acronyms see Table S 2-5 in the Supporting Information.

Text S 2-1: Shuttleworth-Wallace equations as implemented in PMF

$$\lambda ET = C_c\, ET_c + C_s\, ET_s \tag{B.1}$$

where ET is the evapotranspiration [mm d^{-1}], λ is the latent heat of water vaporization [MJ kg^{-1}], ET_c and ET_s are equivalent to transpiration and evaporation using the Penman-Monteith equation for closed canopy and bare soil [MJ $m^{-2}d^{-1}$], C_c and C_s are weighting factors [-]:

$$C_c = 1/(1+ (R_c R_a) / [R_s(R_c+R_a)]) \tag{B.2}$$

$$C_s = 1/ (1+ (R_s R_a)/[R_c(R_s+R_a)]) \tag{B.3}$$

where R_a, R_s and R_c are defined as follows:

$$R_a = (\Delta+\gamma) r_a^a \tag{B.4}$$

$$R_c = (\Delta+\gamma) r_a^c + \gamma\, r_s^c \tag{B.5}$$

$$R_s = (\Delta+\gamma) r_a^s + \gamma\, r_s^s \tag{B.6}$$

where Δ represents the slope of saturation vapor pressure curve [kPa °C^{-1}], γ the psychrometric constant [kPa °C^{-1}], r_a^s and r_a^a are aerodynamic resistances from soil surface to canopy and from canopy to measurement height, r_s^s is the resistance of the soil surface, r_a^c is the bulk boundary layer resistance and r_s^c is the stomatal resistance. All resistances are given in [s m^{-1}].

Text S 2-2: Objective functions

We decided to use several objective functions capable of describing different model performances (Legates and McCabe Jr., 1999; Vis et al., 2015). To evaluate whether the model depicts the right timing of simulations we applied the coefficient of determination (worst, $0 \leq r^2 \leq 1$, best), a criterion that is for example appropriate when evaluating the relationship between soil moisture and rainfall. Since r^2 does not account for under- or overestimation, we selected the bias as a second objective function ($-\infty \leq \text{bias} \leq +\infty$), which is particularly helpful to estimate a model's behaviour in predicting total biomass production over the year. Underestimation is expressed by negative values, overestimation with positive and no bias with bias = 0. Finally, the RMSE (root mean squared error) completed the set of chosen objective functions by providing a measure of differences between simulated and associated observed data, varying from 0 (perfect fit) to large positive values (large disagreement). This third criterion is often used (Moot et al., 2015; O'Leary et al., 2015; Pequeno et al., 2014).

Text S 2-3: Multiple GLUE analysis

For the ambient rings, the GLUE resulted in three posterior parameter sets. These sets contained similar parameter values, i.e. the parameter ranges could be narrowed. Taking the adapted parameter ranges, the GLUE (Table 2-2) was conducted a second time, resulting in 172 parameter sets for the ambient rings.

For the elevated rings, the parameter list was extended by parameter *p* (eq. 2-4) and *b* (eq. 2-5). Using LH sampling 100 parameter sets were generated for *p* and *b*. Every parameter set of the 172 ambient sets was then extended by the 100 combinations of *p* and *b*. Hence, 17,200 parameters sets were generated and taken for the GLUE for the eCO_2 rings. Based on the output the parameter range of *b* was narrowed and a second GLUE was run. The results showed 1398 posterior parameter sets for the rings E1 and E3, but no common sets for all elevated rings. Hence, ring E2 was excluded in the further analysis.

In summary, the overlap of parameter sets of ambient and elevated rings resulted in 82 parameter sets for the ambient and in 1398 for the elevated rings (i.e. 82 sets extended by several *p*-*b*-combinations).

3 Response of maize biomass and soil water fluxes on elevated CO_2 and drought - from field experiments to process-based simulations

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Abstract

The rising concentration of atmospheric carbon dioxide (CO_2) is known to increase the total aboveground biomass of several C3 crops, whereas C4 crops are reported to be hardly affected when water supply is sufficient. However, a free-air carbon enrichment (FACE) experiment in Braunschweig, Germany, in 2007 and 2008 resulted in a 25% increased biomass of the C4 crop maize under restricted water conditions and elevated CO_2 (550 ppm). To project future yields of maize under climate change, an accurate representation of the effects of eCO_2 and drought on biomass and soil water conditions is essential. Current crop growth models reveal limitations in simulations of maize biomass under eCO_2 and limited water supply. We use the coupled process-based hydrological-plant growth model CMF-PMF (Catchment Modelling Framework-Plant growth Modelling Framework) to overcome this limitation. We apply the coupled model to the maize-based FACE experiment in Braunschweig that provides robust data for the investigation of combined CO_2 and drought effects. We approve hypothesis I that CO_2 enrichment has a small direct fertilizing effect with regard to the total aboveground biomass of maize and hypothesis II that CO_2 enrichment decreases water stress and leads to higher yields of maize under restricted water conditions. Hypothesis III could partly be approved showing that CO_2 enrichment decreases the transpiration of maize, but does not raise soil moisture, while increasing evaporation. We emphasize the importance of plant specific CO_2 response factors derived by use of comprehensive FACE data. By now, only one FACE experiment on maize is accomplished applying different water levels. For the rigorous testing of plant growth models and their applicability in

climate change studies, we call for data sets that go beyond single criteria (only yield response) and single effects (only elevated CO_2).

3.1 Introduction

The increase of atmospheric CO_2 has various effects on the soil-plant system. C3 plants show an accelerated CO_2 assimilation rate under elevated CO_2 (eCO_2), which is linked with an increase in biomass production (Ghannoum et al., 2000). In contrast to that, the photosynthesis of C4 plants is reported to be saturated under ambient CO_2 (aCO_2) conditions (Ghannoum et al., 2000). Free-air carbon dioxide enrichment (FACE) experiments are conducted to investigate the effect of eCO_2 under field conditions (Ainsworth & Long, 2004; Hendrey & Kimball, 1994; Leakey et al., 2009; Saban, Chapman, & Taylor, 2019). A number of FACE experiments have been accomplished for C3 plants showing a significant increase in biomass under eCO_2 of 10-15% caused by a CO_2-fertilizing effect (Andresen et al., 2018; Bernacchi et al., 2005; Weigel & Manderscheid, 2012). An average increase of up to 20% in the aboveground biomass was reported by Ainsworth and Long et al. (2004), who conducted a meta-analysis study with 29 different C3 crops and tree species at various FACE experiments. C4 plants such as maize and sorghum however do not respond with an accelerated biomass production under sufficient water supply. This was observed in two FACE experiments on maize in Illinois, USA, and in Braunschweig, Germany and in a FACE experiment on sorghum in Arizona, USA (Leakey, 2006; Manderscheid et al., 2014; Ottman et al., 2001). However, in the unique maize FACE experiment in Braunschweig also the combined effect of eCO_2 and reduced water supply on the C4 crop was tested. The experiment showed a distinct CO_2-induced increase in biomass (+25%) under limited water supply (Manderscheid et al., 2014). A distinct, though weaker (+15%) increase in biomass at harvest was also observed for sorghum under eCO_2 and water stress (Ottman et al., 2001). A water saving effect caused by stomatal closure under eCO_2, that led to an advantage in drier periods, where the maize plants could use the saved water for biomass production was assumed by Manderscheid et al. (2014) and Ottman et al. (2001). Accompanying sap flow measurements in Braunschweig indicated a 20%-reduction of transpiration under eCO_2, caused by increased stomatal resistance under sufficient and restricted water supply (Manderscheid et al., 2016). Saved water by reduced transpiration under eCO_2 increases soil moisture and might further lead to an increase in evaporation (Manderscheid et al., 2018).

To project future yields under climate change, models with a correct response to CO_2 are needed. Tubiello et al. (2007) find that most simulations of established crop models are in agreement with observations of up to date FACE experiments. Jin et al. (2018) simulated successfully the combined effect of eCO_2 and drought for the C3 crop soybean. However, a recent study by Durand et al. (2017) revealed limitations in accurate simulations of biomass of the C4 crop maize under eCO_2 and restricted water supply. The performance of

21 maize crop models was tested against data of the aforementioned two-year FACE experiment with maize in Braunschweig, Germany (Durand et al., 2017). The models reproduced only 30% of the measured, strong biomass increase, and failed to simulate the very low soil moisture values at anthesis (Durand et al., 2017), even though five of the 21 maize models included a sophisticated soil hydrology module based on the Richard equation (Bassu et al., 2014). Plant growth, e.g. biomass accumulation, is slowed and ceased when water stress occurs (Hammer et al., 2010). The effect of water stress is commonly simulated based on either the ratio of actual and potential transpiration, the ratio of water supply and water demand, or the soil moisture content (Jin et al., 2016). To improve the maize models, Durand et al. (2017) emphasized the need for a better representation of the strong reduction of transpiration under eCO_2, to allow a stronger benefit of eCO_2 in periods of water stress. They emphasized in particular, these models must explicitly represent the stomatal response to eCO_2. Fu et al. (2016) applied a single model to a drought / eCO_2 experiment with sorghum, but they have investigated the effects independently and not in combination.

To move forward, accurate CO_2 response functions that describe the reaction of the plant stomata and the plant biomass accumulation to eCO_2 are needed and should be calibrated with recent FACE data. Morison (1987) reviewed 23 studies where the effect of eCO_2 on the plant stomata of different C3 and C4 crops was investigated in lab and open top chamber experiments. Here, a linear increase of the stomatal resistance was observed (Morison, 1987). The doubling from 330 ppm to 660 ppm CO_2 resulted in a 40% increase (Morison, 1987). These effects were implemented in the EPIC model using a simple linear response function with a response factor $p = 0.4$, to account for the 40% change in the stomatal resistance of plants (Stöckle, 1992). Later, the stomatal response factor was specified for C3 ($p = 0.24$) and C4 ($p = 0.29$) pastures based on results of open top chamber and FACE experiments (Wand et al., 1999). In a recent study, where the CO_2 effect on C3 grassland was analysed by the use of a coupled hydrological-plant growth model and long-term data of a FACE experiment on C3 grass, p led to best results when $p = 0.3$ (Kellner et al., 2017). For describing the effect of eCO_2 on net assimilation Goudriaan et al. (1984) presented a simple response function. This was applied by Soltani and Sinclair (2012) to describe the effect of eCO_2 on the radiation use efficiency rue_{CO2}. In this function, a response factor b, which controls the change in rue_{CO2} under eCO_2, was reported to be 0.8 for C3 plants and 0.4 for C4 plants. The study by Kellner et al. (2017) revealed values for $b < 0.3$ for a C3 grassland using long-term FACE data. Both CO_2 response factors have not been calibrated yet using field data of maize.

In this study, we apply the coupled process-based hydrological-plant growth model CMF-PMF, Catchment Modelling Framework (Kraft et al., 2011; Kraft et al., 2018) and Plant growth Modelling Framework (Multsch et al., 2011). To overcome the maize model limitations revealed by Durand et al (2017), we calibrate and validate the model, including the aforementioned two CO_2 response factors for stomatal conductance (p) and biomass accumulation (b) using the data of the maize FACE experiment in

Braunschweig, Germany. We investigate the combined effect of eCO_2 and different soil moisture conditions on the C4 crop maize and identify the important processes for the simulation of CO_2 effects under sufficient and restricted water supply. We test the following hypotheses:

Hypothesis I *eCO_2 has a small direct fertilizing effect with regard to the total aboveground biomass of maize.*
Hypothesis II *eCO_2 decreases water stress and leads to higher yields of maize under restricted water supply only.*
Hypothesis III *eCO_2 reduces the transpiration of maize, increases soil moisture and evaporation.*

We acknowledge that these hypotheses or parts of them have been proven already in experimental trials. However, current model approaches show evident limitations in reflecting the combined effect of water stress and elevated CO_2 on maize production, indicating that those models underestimate the CO_2-fertilizing effect on maize under drought (Durand et al., 2017). This is all the more surprising considering that maize is the most cultivated agricultural crop in the world and that agricultural relevant droughts are projected to occur more frequently and severe at least in Europe (Samaniego et al., 2018). Realistic plant growth models are therefore essential for predicting the effects of climate change on the future production of maize.

3.2 Material and Methods

3.2.1 Data and study site

In this study, data from a FACE experiment in Braunschweig (longitude: 10.45, latitude: 52.29, 81 m a.s.l.), Germany, was used. Maize (*Zea mays* L., cv. Romario) was grown under ambient (aCO_2 = 380 ppm) and elevated carbon dioxide concentrations (eCO_2 = 550 ppm) in 2007 and 2008. In addition to different CO_2 levels, maize was cultivated under two levels of water supply using a combination of irrigation and rainout shelters in one half of each FACE ring. The soil at the study site was a *Luvisol* with loamy sand in the upper 40 cm and sandy gravel below (Manderscheid et al., 2014).

The maize was sown in spring (April/May) and harvested in autumn (September/October) and fertilized with 171 kg N/ha and 198 kg N/ha in 2007 and 2008. CO_2-fumigation started in June and was stopped at harvest. More details of the setup and the management measures of the experiment are available in the Supporting Information Table S 3-1 and S 3-2 and in Erbs et al. (2012), Manderscheid et al. (2014) and Weigel et al. (2005).

Daily sum of precipitation, solar radiation, and daily minimum and maximum of temperature as well as wind speed were measured by the German Meteorological Service at the study site and taken as model input

data. The average temperature was 10.4°C in 2007 and 10.3°C in 2008. Water input by natural rainfall and irrigation was 878 mm and 715 mm in the wet treatment in 2007 and 2008, respectively. In the dry treatment, water input was reduced to 835 mm and 552 mm, respectively in 2007 and 2008 by excluding irrigation and partial application of rain shelters. Detailed information about the water supply in the different treatments is available in the Supporting Information Table S 3-2.

Measured total aboveground biomass (hereafter biomass) and soil moisture were used for model evaluation. Soil moisture was measured approximately twice a week using TDR sensors in three different depths (0.0-0.16 m, 0.2-0.4 m and 0.4-0.6 m) from June until harvest in September/October in both years (Manderscheid et al., 2014). Biomass was measured once a month by destructive harvesting.

3.2.2 Coupled hydrological-plant growth model

For the investigation of climate change effects on the agricultural systems, different types of crop models are used. Most commonly, process-based crop models are applied, in which the most important processes of the soil-plant system are represented (Fodor et al., 2017). In this study, the process-based coupled hydrological-plant growth model CMF-PMF was applied to investigate the combined effect of eCO_2 and drought on biomass accumulation and water consumption of the C4 crop maize. The coupled CMF-PMF has already been successfully tested for C3 plants such as wheat and grassland (Houska et al., 2014; Kellner et al., 2017). With the catchment modelling framework CMF individual hydrological models can be set up (Kraft et al., 2011; Kraft et al., 2018). In this study, CMF was applied as a 1-dimensional plot model that calculates the water transport and the dynamic of the soil moisture profile. Water flux was calculated with a daily time step on the basis of the Richards equation (Richards, 1931). Soil hydraulic characteristics were defined using the van Genuchten-Mualem function, including the parameters: soil porosity, the shape parameter of the van Genuchten retention curve (n) and the inverse of water entry potential (α) (van Genuchten, 1980). The modeled soil column of 0.9 m was divided into four blocks (Supporting Information Table S 3-3), each consisting of several layers. While soil porosity was set according to available measured values in the four blocks, the other important parameters of CMF to describe the soil hydraulic properties such as α, n and saturated conductivity (k_{sat}) were considered in the calibration and uncertainty analysis (Table 3-1, Supporting Information Table S 3-3). The chosen hydrological parameters of the lowest block corresponded to a gravel layer according to the study site. Free drainage was chosen as boundary condition for the lowest layer.

PMF is a plant growth modelling framework which can be used to set up plant models (Multsch et al., 2011). Using plant specific parameters, the generic model PMF can be adapted to simulate different crops. Biomass was calculated using daily time steps with the radiation use efficiency concept, where photosynthetically

active radiation is converted into dry biomass (Monteith & Moss, 1977). The total biomass was distributed to plant components which are available in PMF, such as leaves, stem, storage organs and roots. For this, allocation factors which are specific to every development stage were used. The plant development was driven on the basis of growing degree days, calculating a temperature sum according to the thermal time concept (Monteith & Moss, 1977). Water stress was calculated according to Feddes et al. (1978). The water stress factor limited plant growth by reducing above and below ground biomass accumulation. The factor was derived by dividing actual by potential transpiration. The evapotranspiration was calculated with the model for sparse canopies by Shuttleworth and Wallace (1985).

With the implemented CO_2 response functions, the effect of changing atmospheric CO_2 concentrations on the stomatal resistance as well as the daily biomass allocation can be simulated with PMF. The crop specific CO_2 response is taken into account using the crop specific response factors *p* (stomatal response) and *b* (biomass accumulation). The linear CO_2 response function f_{CO2} governed the stomatal resistance and was implemented according to Stöckle (1992) and Wu et al. (2012):

$$f_{CO2} = (1 + p) - p \cdot CO_{2meas}/CO_{2ref} \qquad \text{eq. 3-1}$$

where CO_{2meas} is the measured atmospheric CO_2 concentration [ppm], CO_{2ref} is the reference CO_2 concentration (here 380 ppm) and *p* is the dimensionless stomatal response factor. The factor *p* ranges between 0 and 1. An increase in *p* results in an increase of the stomatal resistance.

The CO_2 response function of the biomass rue_{CO2} was applied according to Soltani and Sinclair (2012):

$$rue_{CO2} = rue_{ref} \cdot \left(1 + b \cdot \ln\left(CO_{2meas}/CO_{2ref}\right)\right) \qquad \text{eq. 3-2}$$

where rue_{ref} is the radiation use efficiency at 380 ppm which converts photosynthetic active radiation into dry biomass [g MJ^{-1}] and *b* is the dimensionless response factor. The factor *b* ranges between 0 and 1, where $b = 0$ means no increase in rue_{CO2} under eCO_2 and thus no increased biomass accumulation. Since C4 plants react less to eCO_2 than C3 plants, *b* is supposed to be smaller for C4 plant in comparison to C3 plants (Goudriaan et al., 1984).

The two models were coupled using the Python programming language. Running the coupled model, PMF calculated the evapotranspiration and the biomass accumulation including leaf development on time step *t*, taking into account the states of CMF at the prior time step *t*-1. Then, CMF proceeded considering the simulated plant water demand and the leaf area for calculating intercepted precipitation. Further information of the coupled hydrological-plant growth model CMF-PMF are available in Kellner et al. (2017).

For model calibration, eleven plant specific parameters of PMF were used, including three biomass allocation factors ($leaf_{leafdev}$, $leaf_{stemelong}$, $shoot_{leafdev}$), the minimum temperature for plant development (t_{base}),

the temperature sum for emergence ($tt_{emergence}$), the reference radiation use efficiency at 380 ppm CO_2 (rue_{ref}), the specific leaf weight ($leaf_{weights}$), the leaf extinction coefficient for the calculation of the net radiation (c_r), the minimum stomatal resistance of leaves, which is relevant to transpiration (r^{st}_{min}), and the two CO_2 response factors *p* and *b* (Table 3-1).

3.2.3 Model calibration, validation and uncertainty analysis

To avoid overfitting and to investigate parameter uncertainty, we were not optimizing to find one best parameters set during the calibration period, but applied a rejectionist Monte Carlo approach and followed the concept of equifinality, where several parameter sets can result in equally adequate model runs (Beven & Binley, 1992). The model was calibrated using the data of the FACE rings under aCO_2 and eCO_2 in 2007, where only a small difference in water supply occurred. The calibration approach followed the scheme outlined in Figure 3-1. The model was validated by comparing simulations with the final parameter sets with field measurement of the wet and dry, aCO_2 and eCO_2 treatments in 2008.

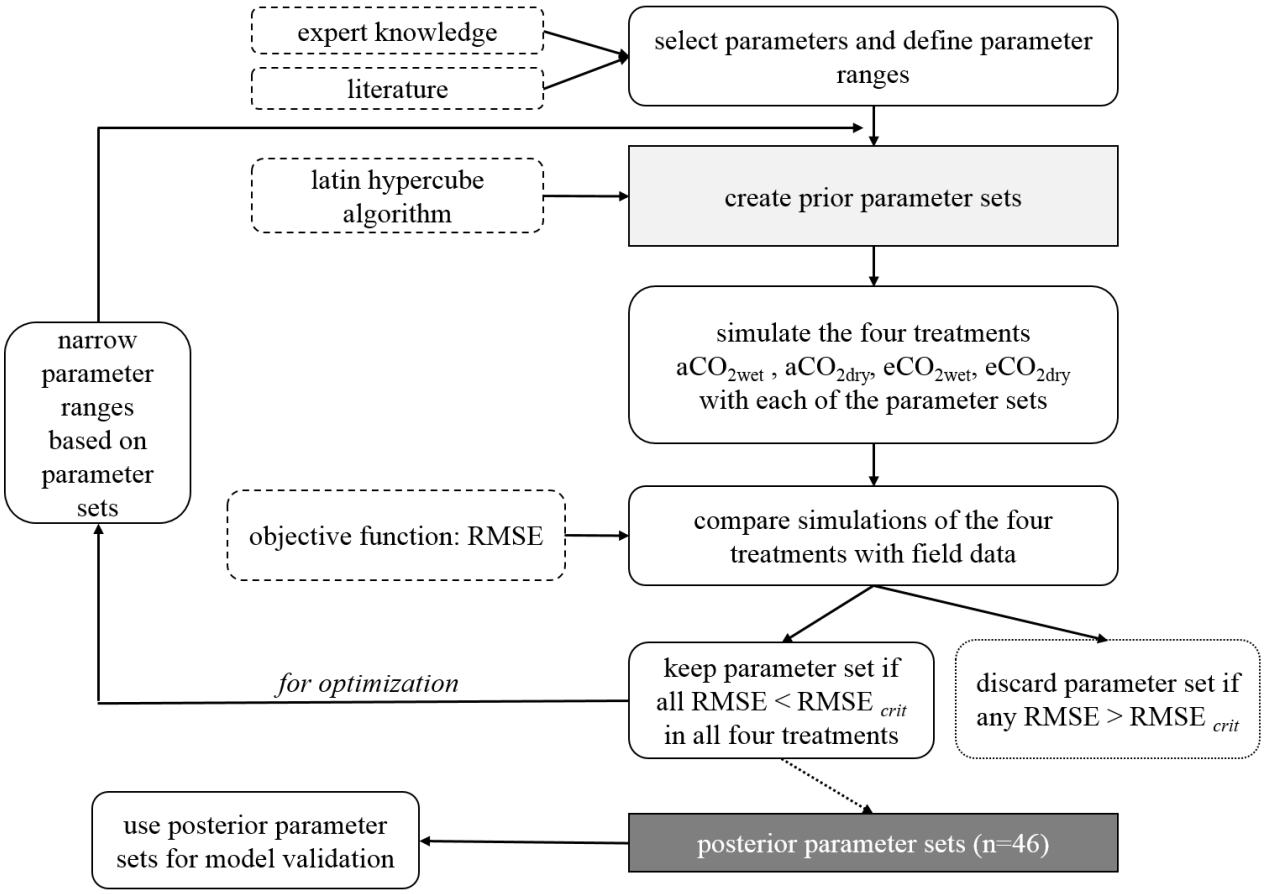

Figure 3-1: Flow chart of the conducted model calibration approach. For reasons of optimization the prior parameter ranges were iteratively narrowed. Finally, 46 posterior parameter sets for all four treatments in the FACE experiment in Braunschweig in maize 2007 were identified.

Based on literature values and expert knowledge three CMF and eleven PMF parameters were selected and an upper and a lower limit was set for every parameter (Table 3-1). 50,000 parameter sets for the 14 parameters were randomly picked assuming a uniform distribution within the defined ranges and using the latin hypercube algorithm (McKay et al., 1979) as implemented in the SPOTPY package (Houska et al., 2015). Each of the four treatments was then simulated with each of the 50,000 parameter sets. Hereafter, we followed an independent multi-criteria model selection approach (Houska et al., 2017), i.e. we compared simulated and measured biomass and soil moisture data from 2007 as four independent criteria for model calibration. For the evaluation of a model run, the root-mean-squared error (RMSE) was taken as the objective function. $RMSE_{crit}$ thresholds were defined as <6 vol.% for soil moisture and $RMSE_{crit}$ <1.30 Mg ha^{-1} for biomass. Only model runs that resulted in all four treatments of 2007 in smaller RMSE values than the user-defined thresholds of $RMSE_{crit}$ were further considered. In this study, we conducted the rejectionist-based Monte Carlo approach iteratively to optimize the simulations. For this, the parameter ranges were adapted based on the results of the previous model run. Parameter sets were randomly picked using latin hypercube sampling. The posterior parameter ranges are listed in Table 3-1. Posterior parameter sets were validated by using biomass and soil moisture data of 2008.

Table 3-1: Parameter ranges of the 14 parameters as used in the uncertainty analysis. Listed are the prior ranges at the beginning of the analysis and the final ranges that was found in the 46 posterior parameter sets.

parameter	**description and unit**	**prior ranges**		**posterior ranges**	
		Min	**Max**	**Min**	**Max**
soil hydraulic parameters (CMF)					
α	inverse of the air entry potential, empirical [cm^{-1}]	0.01	0.70	0.02	0.04
k_{sat}	saturated conductivity [m day^{-1}]	0.1	12	5	6
n	shape parameter of the van Genuchten retention curve, empirical [-]	1.1	1.5	1.4	1.5
plant specific parameters (PMF)					
b	CO_2 response factor of rue [-]	0	1	0	0.3
c_r	leaf extinction coefficient [-]	0.1	0.8	0.6	0.8
$leaf_{leafdev}$	leaf biomass allocation factor during leaf development [-]	0.70	0.95	0.70	0.95
$leaf_{stemelong}$	leaf biomass allocation factor during stem elongation [-]	0.3	0.5	0.3	0.4
$leafweight_s$	specific leaf weight [g m^{-2}]	20	110	80	110
p	CO_2 response factor of stomata [-]	0	1	0.7	1
r^{st}_{min}	min stomatal resistance of individual leaves under optimum conditions [s m^{-1}]	40	130	110	130
rue_{ref}	radiation use efficiency at 380 ppm CO_2 [g MJ^{-1}]	3.0	4.5	3.9	4.0
$shoot_{leafdev}$	shoot biomass allocation factor during leaf development [-]	0.4	0.6	0.5	0.6
t_{base}	min temperature for plant growth [°C]	5.0	12.0	5.0	5.5
$tt_{emergence}$	thermal time at emergence [°days]	20	200	80	100

3.3 Results

The rejectionist-based Monte Carlo approach identified 46 parameter sets for accurate simulation of biomass and soil moisture under aCO_2 and eCO_2 in combination with wet and dry conditions in the year 2007. The prior parameters ranges could be narrowed and revealed optima (Supporting Information Figure S 3-2). The coefficient *b* showed only values <0.1, which described a small response of biomass accumulation to eCO_2. Factor *p* was >0.7, which represented a strong increase in stomatal resistance under eCO_2. Radiation use efficiency rue_{ref} at 380 ppm had a maximum at 3.91 g MJ^{-1}. The hydrological parameters *n* and α revealed optimal settings at 1.42 and 0.03 and k_{sat} ranged between 5.2 and 5.6 m day^{-1}.

The coupled hydrological-plant growth model performed well for biomass simulations in all treatments in the calibration year 2007 with an RMSE <1.30 Mg ha^{-1} (Figure 3-2). The accurate model performance was further approved by a not significant difference between simulated and measured biomass ($p > 0.1$ in all treatments in 2007 (Supporting Information Table S 3-4)). On average, the simulated biomass at harvest was 21.2 ±0.3 and 21.3 ±0.2 Mg ha^{-1} under aCO_2 and eCO_2, similar to measured yields of 21.4 ±0.6 and 21.7 ±0.8 Mg ha^{-1}, respectively. Water stress was negligible in all treatments throughout the growing period in 2007 (Supporting Information Figure S 3-3). This resulted in similar yields in 2007, when comparing the wet and dry treatments (Figure 3-3a). In line with the field data, the coupled model simulated no CO_2-induced increase in biomass at harvest in 2007 (measured wet and dry: +2.1 and +0.7%, simulated wet and dry: +0.6 and +0.6%, Figure 3-3b).

In the validation year 2008, results of the hydrological-plant growth model showed slightly higher RMSEs. In the wet treatment, the RMSE was below 1.2 and 1.7 Mg ha^{-1} under aCO_2 and eCO_2 for the biomass simulations. There was no significant difference observed between measured and simulated biomass in the wet treatment 2008 ($p > 0.1$, Supporting Information Table S 3-4). The model simulated again no relevant CO_2-induced biomass increase in the wet treatment (+1.3%) which was in agreement with field observations (-1.0%). Simulated biomass at harvest was 22.9 ±0.6 and 23.2 ±0.6 Mg ha^{-1} under aCO_2 and eCO_2 in the wet treatment. Similar biomass yields were measured in the field with 23.0 ±0.1 and 22.8 ±1.0 Mg ha^{-1} (Figure 3-3a). However, in the dry treatment a significant increase of +20% in biomass was simulated (Kruskal-Wallis test: $p < 0.01$). A marked biomass response was also observed under eCO_2 with +25% in the dry treatment in 2008 (Figure 3-3b). The measured biomass under eCO_2 was statistically slightly different from the simulated biomass ($p = 0.024$). The simulated water stress, which occurred during the growing period, was distinctly reduced by -37% under eCO_2 from middle of July to harvest (Supporting Information Table S 3-3).

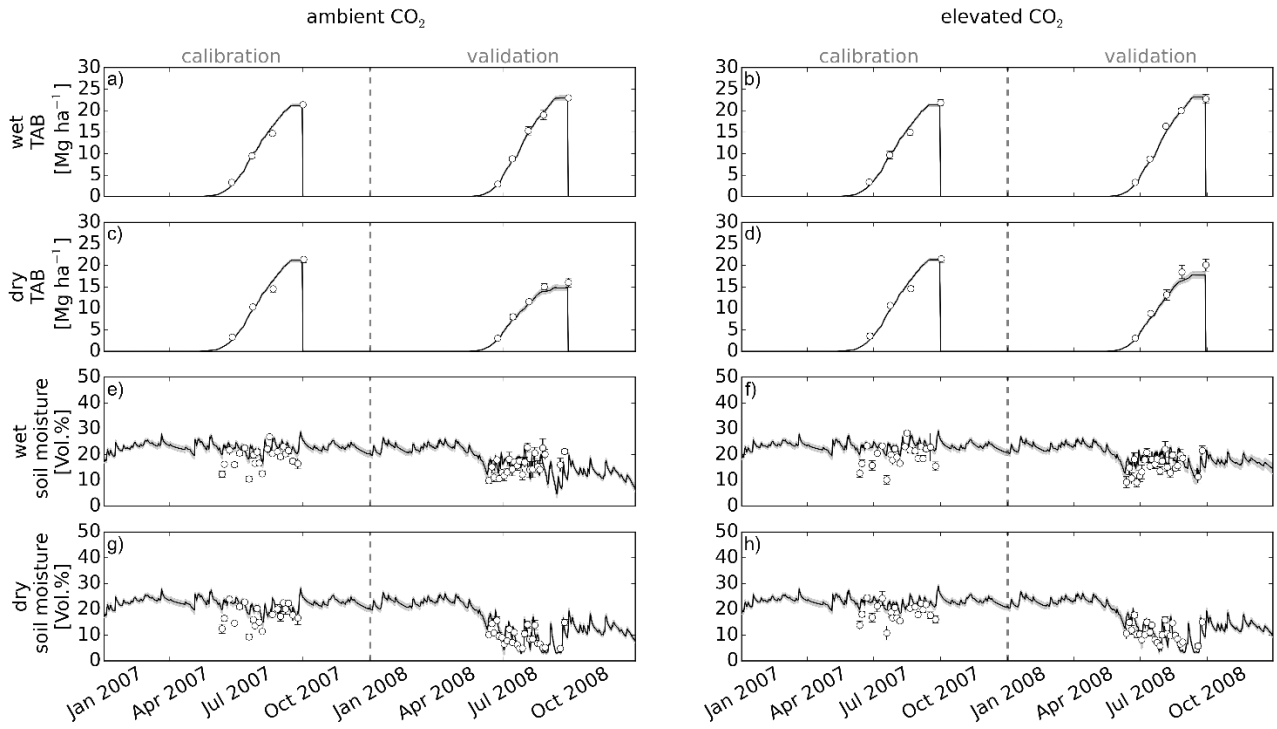

Figure 3-2: Time series of biomass and soil moisture in the different treatments: wet, dry, aCO_2 and eCO_2; a-d) mean total aboveground biomass (TAB), and e-h) mean soil moisture in 0-0.16 m depth with standard deviation of the Braunschweig FACE rings with maize. Measured values = dots, simulated = solid line, aCO_2 = a), c), e) and g), eCO_2 = b), d), f) and h). The number of posterior parameter sets was n = 46 (shaded area around the mean).

In addition to the biomass, the CMF-PMF adequately simulated the course of the measured soil moisture in all treatments in 2007, showing an RMSE <6 vol.% (Figure 3-2). In the dry treatment, the simulated soil moisture for the depth 0-0.6 m was on average 19.3 ±2.1 and 20.9 ±1.5 vol.% under aCO_2 and eCO_2, while observations were only slightly smaller with 18.9 ±4.6 and 20.3 ±4.2 vol.%, respectively (Supporting Information Figure S 3-1). In the wet treatment, the simulated soil moisture was on average 20.6 ±1.8 and 21.4 ±1.5 vol.% under aCO_2 and eCO_2. This was in agreement with the measurements, where the soil moisture was 19.4 ±4.7 and 21.2 ±4.0 vol.%. The model simulated no CO_2-induced change in soil moisture (dry: +1.6 vol.%, wet: +0.8 vol.%), which was in line with the observed data (dry: +1.4 vol.%, wet: +1.8 vol.%). Minor deviations between observations and simulations should also been seen from the aspect of the measurement accuracy of 1-2% of the soil moisture sensors used.

In the validation period 2008, the model uncertainty was small, with RMSEs below 6 and 7 vol.% in the wet and dry treatment, respectively. Especially, in the dry treatment in 2008, the model showed a good model performance and reproduced the measured low (around 10 vol.%) and higher soil moistures (around 20 vol.%), especially in the upper 0.16 m of the soil column (Figure 3-2). In 2008, the coupled model

simulated an average soil moisture for the depth 0-0.6 cm of 15.0 ±2.9 and 16.9 ±2.0 vol.% in the wet, and 9.2 ±4.3 and 10.3 ±4.1 vol.% in the dry treatment under aCO_2 and eCO_2, respectively. Observed soil moistures were in the same ranges with 16.7 ±3.6 and 17.8 ±3.2 vol.% (wet) and 10.6 ±4.0 and 13.1 ±3.9 vol.% (dry) under aCO_2 and eCO_2. Under eCO_2 the hydrological-plant growth model simulated no increase in soil moisture beyond the measurement accuracy (wet: +1.9 vol.% and dry: +1.1 vol.%). Likewise in the measurements no change in soil moisture was observed under eCO_2 (wet: +1.1 vol.% and dry: +2.5 vol.%).

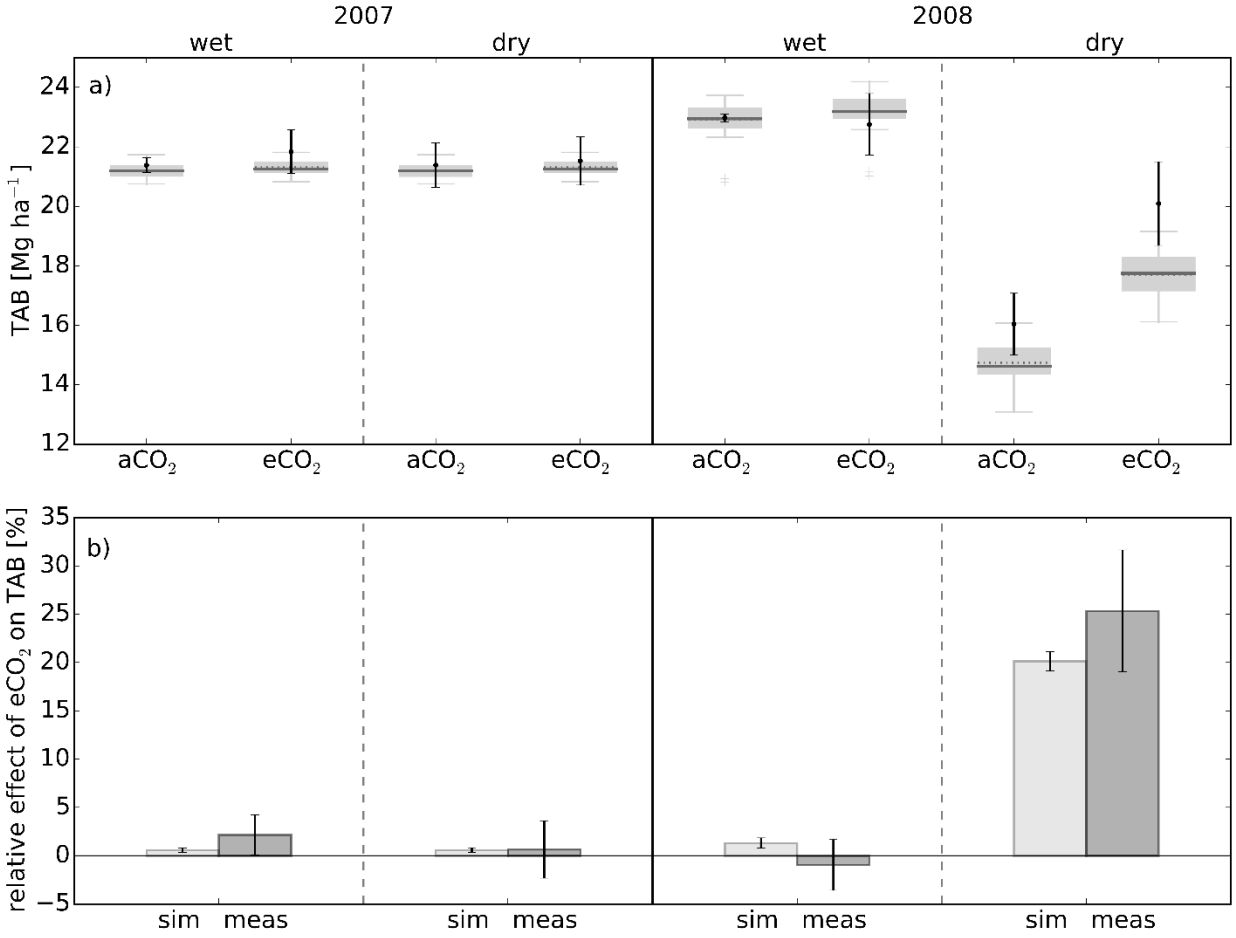

Figure 3-3: Simulated and measured biomass in the wet and dry treatment in 2007 and 2008 in Braunschweig, Germany. a) Absolute total aboveground biomass (TAB) of maize [Mg ha^{-1}] at harvest; gray boxes include 50% of the model runs and error bars include 90% of the model runs, median = solid line, mean = dotted line; black dots indicate mean of measured data, error bars show the standard deviation; b) Simulated (light gray) and measured (gray) relative impact of eCO_2 on TAB of maize [%] at harvest, error bars indicate the relative standard deviation of the difference between the simulated means.

CMF-PMF simulated a significant ($p<0.05$) reduction of the evapotranspiration under eCO_2 in 2007 by -15% (wet and dry) and in 2008 by -14% (wet) and -2% (dry) during the respective growing period of maize. The simulated transpiration was reduced by -22% (dry and wet 2007, wet 2008) and -6% (dry 2008). In turn, the

evaporation increased under eCO_2 by +8% in 2007 and by +12.5% and +10.4% in 2008 in the wet and dry treatment (Figure 3-4).

The water use efficiency (WUE) was calculated by dividing the biomass at harvest by accumulated evapotranspiration from sowing to harvest. In both years a significant ($p < 0.01$) increase in WUE was simulated under eCO_2. The strongest enhancement occurred in the dry treatment in 2008 (+22.0%) compared to +17.4% in the wet treatment 2008 and +17.8% in both setups in 2007 (Figure 3-4, Supporting Information Table S 3-5).

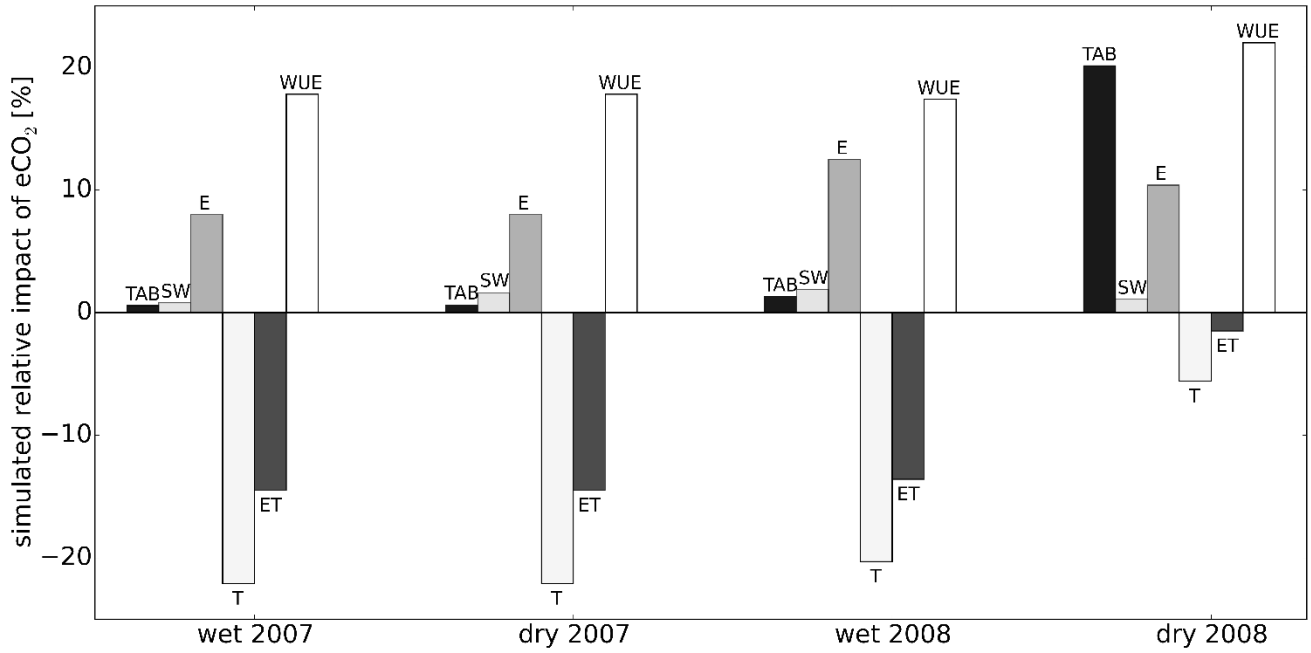

Figure 3-4: Simulated relative impact of eCO_2 [%] in the wet and dry treatments in 2007 and 2008 on total aboveground biomass (TAB), soil moisture (SW), evaporation (E), transpiration (T), evapotranspiration (ET) and water use efficiency (WUE).

3.4 Discussion

3.4.1 Model performance

For investigating the combined effect of eCO_2 and different water supply on the C4 crop maize we applied the coupled hydrological-plant growth model CMF-PMF. To identify the values of the implemented CO_2 response factors, the model was calibrated under ambient and elevated CO_2 conditions using data from the maize FACE experiment in Braunschweig, Germany in 2007 (Manderscheid et al. 2014). For model validation, we used data of the consecutive year 2008. The model performance was evaluated using RMSE.

The RMSE of the biomass simulations was very small in 2007 with 1.3 Mg ha^{-1} for all treatments. In 2008, the RMSE was around 1.7 Mg ha^{-1} in the wet treatment and 2.4 Mg ha^{-1} in the dry treatment. This performance was good compared to other published studies. Cavero et al. (2000), who evaluated the EPICphase model using field data of a maize experiment under restricted water conditions in Zaragoza, Spain, reported for instance an RMSE of 3.8 Mg ha^{-1}. Durand et al. (2017) estimated a mean RMSE of 2.1 Mg ha^{-1} when simulating biomass at harvest of the FACE maize in Braunschweig in 2007 and 2008 with an ensemble of 21 crop models. The RMSE of the soil moisture was <6% in 2007 and <7% in 2008 all treatments. A similar performance has been shown in other studies. Saseendran et al. (2005) calculated an RMSE between 5 to and 9% using CERES-Maize model, when comparing simulated soil moisture with measurements of a field experiment with three maize hybrids in Colorado, US. Eitzinger et al. (2004) found RMSEs of soil water content between 1 and 7% comparing simulated soil moisture of the CERES-Wheat model with observed soil moisture in a field experiment with wheat and barley on different soils in Marchfeld, Austria.

3.4.2 Hypothesis I: CO_2 has a small fertilizing effect regarding biomass accumulation of maize

We tested hypothesis I that CO_2 enrichment only has a small direct-fertilizing effect with regard to the biomass of maize. This hypothesis could be approved. In 2007, there was no increase in either simulated or measured biomass. The absence of a fertilizing effect of eCO_2 was also visible in the wet treatment of the validation year 2008. We were able to simulate the absence of a CO_2 effect by calibrating the CO_2 response factor of the biomass accumulation. This factor controls the plant biomass increase under eCO_2 by changing the radiation use efficiency. Under aCO_2 (=380 ppm) the calibrated radiation use efficiency rue_{ref} ranged between 3.9 and 4.0 g MJ^{-1}. Stöckle et al. (1992) reported a similar value of 3.9 g MJ^{-1} for maize under 350 ppm. Lindquist et al. (2005) suggested a rue_{ref} of 3.8 g MJ^{-1} for yield prediction under optimum conditions. For the simulation of a potential CO_2 effect, rue_{ref} was adapted using factor b (see eq. 3-2). In this study, b was <0.1 in all final 46 parameter sets. This was low compared to former reported values of 0.4 for C4 plants (Goudriaan et al., 1984) and 0.3-0.8 for C3 plants (Goudriaan et al., 1984, Kellner et al., 2017). However, maize biomass accumulation was not stimulated by eCO_2 as observed in the FACE experiment in Braunschweig (Manderscheid et al., 2014) and in the maize FACE experiment in the US (Leakey, 2006). Hence, for simulating the absence of the CO_2 effect b needed to be small. Applying eq. 3-2 with rue_{ref} = 4.0 g MJ^{-1} and b = 0.1, the increase of about 170 ppm CO_2 led to a maximum rise of the radiation use efficiency under eCO_2, rue_{CO2}, to 4.1 g MJ^{-1}. This in turn did not increase simulated biomass.

Hence, simulating the absence of a CO_2 effect could be realized by calibrating and reducing the reported CO_2 response factor with field data of the Braunschweig FACE experiment on maize.

3.4.3 Hypothesis II: CO_2 enrichment decreases water stress and leads to higher yields of maize under dry conditions

Further, we tested hypothesis II that CO_2 enrichment decreases water stress and leads to higher yields of maize under dry conditions only. This hypothesis could be approved as well. In 2007, there was no water stress simulated. However, water stress occurred in the dry treatment in 2008. In line with the field data, this led to a decreased biomass accumulation compared to the wet treatment. However, the water stress was significantly reduced under eCO_2 (-37%). The reason for the strong reduction of water stress was a simulated increased stomatal resistance under eCO_2. Factor *p*, which controls the change in stomatal response under eCO_2, was >0.7 in all 46 final parameter sets, which represents a 70% increase in stomatal resistance. This was higher than the reported values of former studies, where *p* was 0.4 for C4 plants based on literature review (Morison, 1987), 0.29 for C4 pastures based on a meta-analysis (Wand et al., 1999) and 0.3 for a C3 dominated grassland (Kellner et al., 2017). However, the linked reduced water stress allowed the plants to accumulate more biomass under eCO_2 compared to aCO_2. In line with this, our model succeeded in showing a distinct response of biomass to eCO_2 under restricted water supply (+20%) in 2008. The simulated biomass increase was 5% lower than the observed increase in the field experiment (+25%). However, it was significantly higher than the response of the model ensemble of 21 maize crop models, which resulted in an increase of biomass of only 11% when applying the model ensemble to the FACE data of Braunschweig (Durand et al., 2017). In line with Durand et al. (2017), we emphasize the importance of an explicit stomatal control on transpiration in crop models. This enables the simulation of a strong CO_2 response under dry conditions and facilitates to project reduced water stress. We emphasize the importance of up to date FACE data for calibrating CO_2 response factors. Further optimization of the model, might be achieved by including for instance CO_2 effects on plant architecture and partitioning between roots and shoots as indicated by Fodor et al. (2017). Anyway, more FACE experiments with maize under wet and dry conditions are needed to identify missing responses in recent crop models.

3.4.4 Hypothesis III: CO_2 enrichment reduces the transpiration of maize and hence, increases soil moisture and evaporation

The third hypothesis tested was that CO_2 enrichment reduces the transpiration of maize and hence, increases soil moisture and evaporation. The reduction of transpiration could be approved, however, a simulated

increase in soil moisture was not found above the measurement accuracy. The evaporation, however, was simulated to increase under eCO_2. An accurate simulation of the transpiration is important, since an underestimated reduction of transpiration hampers the maize model to simulate a strong biomass increase under eCO_2 (Durand et al., 2017). In our study, the simulated transpiration was reduced by 22% in 2007 (wet and dry) and in 2008 (wet). A significant reduction in transpiration of maize has been observed in a FACE experiment in the US, where CO_2 was increased from 376 ppm to 550 ppm (Hussain et al., 2013). Further, Manderscheid et al. (2016) indicated a decrease of transpiration by 20% when deriving transpiration rates from sap flow measurements of the maize in the FACE experiment in Braunschweig 2007 and 2008. In the dry treatment in 2008, the simulated reduction of transpiration under eCO_2 was much smaller with only -6%. The small effect on transpiration was in line with observations by Manderscheid et al. (2016) who reported even no effect of sap flow on the dry treatment in 2008. The reduced water stress led to a significant increase in biomass production. The increased biomass in turn raised water consumption and finally counteracted the expected reduction of transpiration. In total, the evapotranspiration was reduced by -15% in 2007 (wet and dry) and in 2008 by -14% (wet) and -2% (dry). However, despite of an overall decreased water consumption, there was no increase in simulated soil moisture. The absence of increased soil moisture was already indicated by Manderscheid et al. (2014) who reported no significant increase in 2007 in both treatments and 2008 in the wet treatment. However, a significant increase in plant available water was detected on several dates during July and August 2008 in the dry treatment. The evaporation, which mainly depends on the water content and the incoming radiation at soil surface, was simulated to increase by 8-12.5%. The water used for higher evaporation rates origins from the saved water by reduced transpiration under eCO_2. A similar effect was reported by a recent study of Manderscheid et al. (2018), who investigated the effect of eCO_2 (600 ppm) on evapotranspiration and water use of wheat. Finally, the simulated increase in water use efficiency of +22% in the dry treatment in 2008 conformed with an indicated water use efficiency of +25% in the same treatment by Manderscheid et al. (2014). We show an accurate simulation of the CO_2 effect on biomass of the C4 plant maize under wet and dry conditions using the coupled hydrological-plant growth model CMF-PMF. We emphasize the importance of deriving plant specific CO_2 response factors using comprehensive FACE data. For the rigorous testing of plant growth models and their applicability in climate change studies, we call for data sets that go beyond single criteria (only yield response) and single effects (only elevated CO_2). Using such data from the Braunschweig maize experiment, we were able to calibrate the CMF-PMF model independently for ambient and elevated conditions, including an uncertainty assessment. The validation was successful, even though the environmental conditions during the calibration period were significantly different. This supports our assumption that the CMF-PMF captures the relevant plant growth mechanisms induced by climate change. The parameters for the stomatal CO_2 response can be transferred to other models of *Zea mays* growth to predict yields under global change conditions. The change in radiation use efficiency by elevated CO_2 is crucial to model CO_2

response for C3 plants, but should and can be omitted for C4 plants. This provides a simple blueprint to enable existing C4 plant models to include a response to coupled drought / CO_2 effect on yield. The presented methodology is not limited to specific crop type or plant species, but a FACE dataset. We emphasize the need of further FACE studies, especially when dealing with global highly relevant C4 crops, such as maize, sorghum, millet and sugar cane, to enable the modelling community to update and test their process-based crop models.

Acknowledgements

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Supporting Information

Table S 3-1: Key dates of management of the maize crops in the FACE experiment in Braunschweig, Germany, in 2007 and 2008.

	sowing	**harvest**	**CO_2 fumigation**
2007	30 Apr	01 Oct	09 Jun – 29 Sep
2008	09 May	29 Sep	11 Jun – 02 Oct

Table S 3-2: Water supply in the different treatments in 2007 and 2008 including the annual sums of rainfall, rainfall reduction, irrigation and total water input [mm].

year	**rainfall [mm]**	**excluded rainfall [mm]**		**irrigation [mm]**		**total water supply [mm]**	
		wet	dry	wet	dry	wet	dry
2007	844	-	-9	34	-	878	835
2008	609	-	-57	119*, 94**	-	728*, 703**	552

* in aCO_2 rings, ** in eCO_2 rings

Table S 3-3: Definition of soil hydraulic properties for the FACE experiment in Braunschweig as used in in CMF. The parameters k_{sat}, α, n were considered in the uncertainty analysis. The parameters α_2 and n_2 were set to fixed values according to properties of a gravel layer.

block	**depth [m]**	**layers [m]**	**porosity [%]**	**k_{sat} [m day^{-1}]**	**α [-]**	**n [-]**
1	0.0 – 0.2	10 x 0.02	$\Phi_1 = 44$	k_{sat1}	α_1	n_1
2	0.2 – 0.4	5 x 0.04	$\Phi_2 = 40$	$k_{sat2} = 0.66 \cdot k_{sat1}$	α_1	n_1
3	0.4 – 0.8	4 x 0.10	$\Phi_3 = 38$	$k_{sat3} = 0.50 \cdot k_{sat1}$	α_1	n_1
4	0.8 – 0.9	1 x 0.10	$\Phi_4 = 35$	$k_{sat4} = 25.0$	$\alpha_2 = 0.2$	$n_2 = 1.5$

Table S 3-4: Statistical analysis of difference between simulated and measured biomass using the Kruskal-Wallis test, n = sample size.

biomass measured	**biomass simulated**	**n**	**p-value**
2007 aCO_2 wet measured	2007 aCO_2 wet simulated	3/46	0.278
2007 eCO_2 wet measured	2007 eCO_2 wet simulated	3/46	0.278
2007 aCO_2 dry measured	2007 aCO_2 dry simulated	3/46	0.646
2007 eCO_2 dry measured	2007 eCO_2 dry simulated	3/46	0.359
2008 aCO_2 wet measured	2008 aCO_2 wet simulated	3/46	0.835
2008 eCO_2 wet measured	2008 eCO_2 wet simulated	3/46	0.559
2008 aCO_2 dry measured	2008 aCO_2 dry simulated	3/46	0.079 *
2008 eCO_2 dry measured	2008 eCO_2 dry simulated	3/46	0.024 **

Table S 3-5: Mean WUE ±standard deviation [g m^{-2} mm^{-1}] in all treatments. The columns Δ_{wet} and Δ_{dry} show the CO_2-induced difference in WUE [%], two asterisks (**) indicates $p<0.01$, when testing significant difference between WUE under aCO_2 and eCO_2.

	WUE wet treatment			**WUE dry treatment**		
year	**aCO_2**	**eCO_2**	**Δ_{wet}**	**aCO_2**	**eCO_2**	**Δ_{dry}**
2007	5.4 ±0.1	6.4 ±0.2	+17.8**	5.4 ±0.1	6.4 ±0.2	+17.8**
2008	5.0 ±0.1	5.8 ±0.2	+17.4**	4.7 ±0.2	5.7 ±0.3	+22.0**

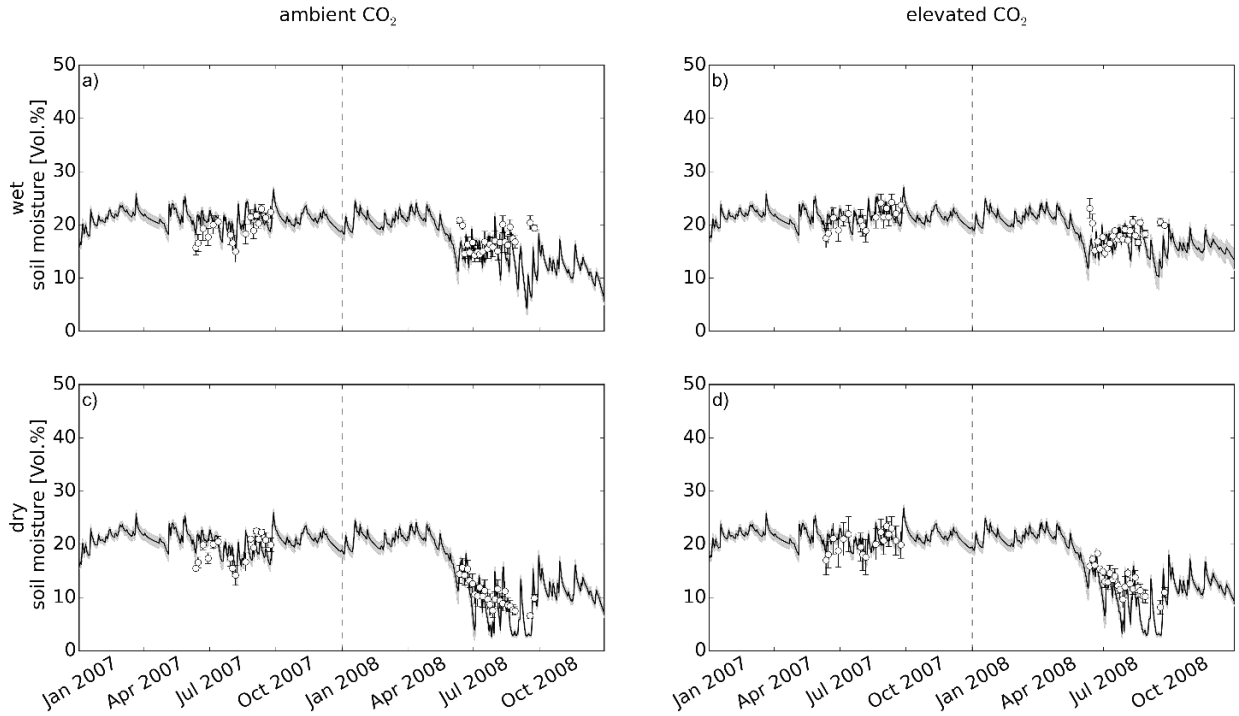

Figure S 3-1: Soil moisture in 0-60 cm depth at the Braunschweig study site. Measured values = dots with standard deviation (n=3) and, simulated values = solid line with standard deviation (n=46), ambient CO_2 = a) and c), elevated CO_2 = b) and d).

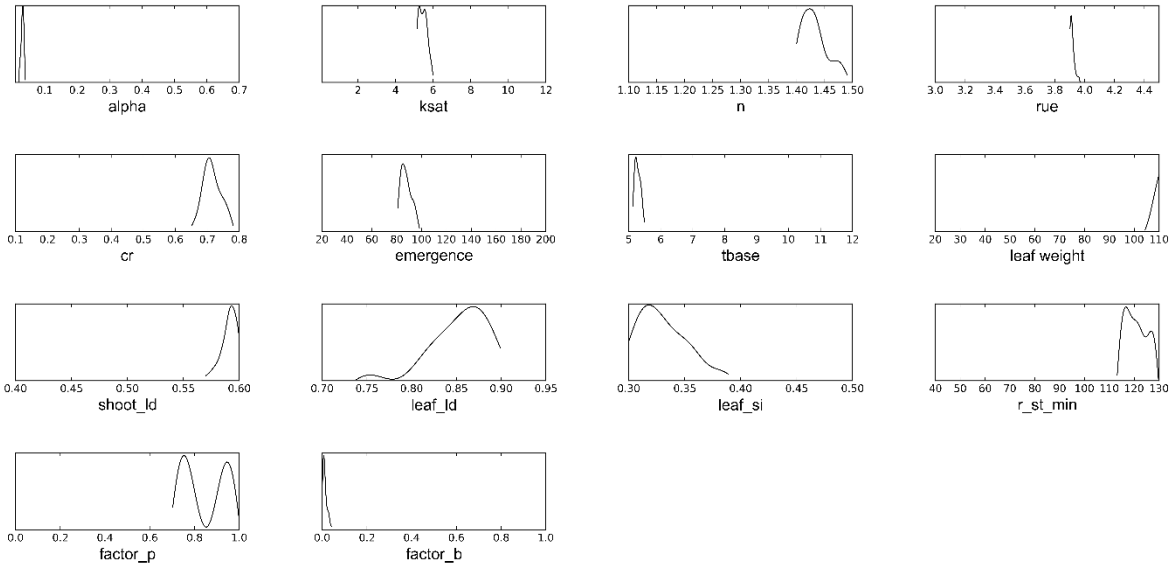

Figure S 3-2: Parameter density distribution of the 46 posterior parameter set using prior ranges.

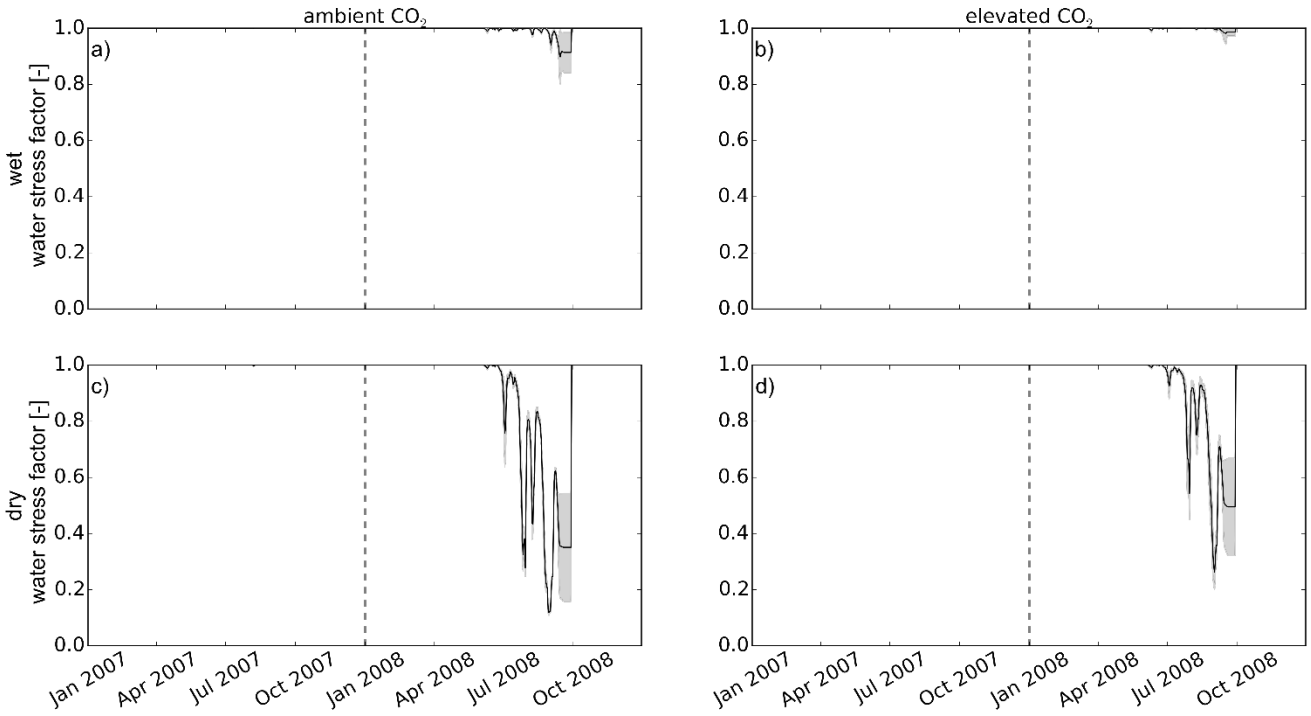

Figure S 3-3: Time series of the simulated water stress factor (0 = full stress, 1= no stress) for the wet treatment (a and b), and the dry treatment (c and d); the solid black line represents the mean water stress factor of the simulations, the grey area indicates the standard deviation (n=46).

Text S 3-1: Relative difference between the means

The difference between the means, $\mu_{e\text{-}a}$ [Mg ha^{-1}], was calculated by $\mu_{e\text{-}a} = \mu_e - \mu_a$ with μ_e = mean of TAB under eCO_2 and μ_a = mean of TAB under aCO_2. The relative difference, $r\mu$ [%], was then $r\mu = \mu_{e\text{-}a} / \mu_e * 100$. The standard deviation of the difference between the means, $r\sigma_{e\text{-}a}$ [%], was calculated by $r\sigma_{e-a} = \sqrt{\frac{\sigma_e^2}{n_e} + \frac{\sigma_a^2}{n_a}} / \mu_a * 100$.

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Declaration

I declare that I have completed this dissertation single-handedly without the unauthorized help of a second party and only with the assistance acknowledged therein. I have appropriately acknowledged and cited all text passages that are derived verbatim from or are based on the content of published work of others, and all information relating to verbal communications. I consent to the use of an anti-plagiarism software to check my thesis. I have abided by the principles of good scientific conduct laid down in the charter of the Justus Liebig University Giessen „Satzung der Justus-Liebig-Universität Gießen zur Sicherung guter wissenschaftlicher Praxis“ in carrying out the investigations described in the dissertation.”

Giessen, 19th August 2019

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Juliane Kellner